

## Article

# A $\Delta$ SCF-DFT Donor–Acceptor Descriptor Map for Main-Group Atoms: Validation, Basis-Set Sensitivity, and Diagnostic Anionic States

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## Abstract

Ionization potentials and electron affinities provide the energetic basis for several conceptual density functional theory descriptors, but their use in donor–acceptor maps requires careful distinction between physically bound anions, weak or borderline electron-affinity cases, and formally computed diagnostic states. In this work, a periodic donor–acceptor descriptor map was constructed for main-group atoms from H to Kr using a  $\Delta$ SCF-DFT framework. Neutral atoms, monocations, and formally defined monoanionic states were evaluated to obtain ionization potentials, electron affinities, and global reactivity descriptors, including electronegativity, chemical hardness, chemical potential, electrophilicity, electrodonating power, and electroaccepting power. The production dataset was calculated at the  $\omega$ B97X-D4/def2-QZVPPD level and benchmarked against reference atomic data. This protocol reproduced ionization potentials with a mean absolute error of 0.134 eV and electron affinities with a mean absolute error of 0.116 eV for the reference EA set, including the weak calcium case. A functional and basis-set sensitivity analysis using  $\omega$ B97X-D4/def2-TZVPPD, PBE0/def2-QZVPPD, and PBE0/def2-TZVPPD showed that ionization potentials are comparatively robust, whereas electron affinities are strongly affected by the quality of the diffuse basis set. The normalized donor–acceptor map reproduces chemically intuitive periodic trends, with alkali metals occupying the strong-donor region and halogens defining the strong-acceptor region. The analysis explicitly separates core validation atoms from weak or borderline electron-affinity cases and diagnostic finite-basis anionic states, emphasizing that formally computed negative electron affinities for unbound anions should not be interpreted as physical bound states. The resulting nonrelativistic dataset provides a reproducible atomic descriptor reference for interpreting donor–acceptor behavior in atoms, clusters, superatoms, doped materials, and charge-transfer systems.

**Keywords:** conceptual DFT; electron affinity; ionization potential; donor–acceptor map; DeltaSCF-DFT



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## 1. Introduction

Atomic ionization potentials and electron affinities are among the most fundamental quantities used to describe the electronic response of atoms [1]. Together, they provide direct information on the tendency of a species to lose or accept electronic charge and therefore underpin several qualitative concepts in chemistry, including electronegativity, hardness, softness, donor–acceptor behavior, and periodic reactivity trends [2]. Because these energetic quantities influence charge transfer, redox behavior, and bonding tendencies,

they also serve as foundational parameters for conceptual density functional theory (DFT) descriptors [3].

Within the framework of conceptual DFT, the ionization potential and electron affinity are mathematically connected to the chemical potential, chemical hardness, and electronegativity [3,4]. These parameters allow the derivation of additional global reactivity indices, including the Parr electrophilicity index, which provides a measure of the electron-accepting tendency of a species [5]. To further distinguish donation and acceptance behavior, Gázquez and coworkers introduced the electrodonating ( $\omega^-$ ) and electroaccepting ( $\omega^+$ ) powers [6]. When applying these descriptors, it is important to note that lower  $\omega^-$  values indicate greater electron-donating capability, whereas larger  $\omega^+$  values indicate stronger electron-accepting character. Together, these quantities provide a useful framework for comparing the reactivity of atoms, molecules, clusters, and materials [7].

Although conceptual DFT descriptors are routinely applied to molecular and solid-state systems, a consistent atomic donor–acceptor reference map remains useful because it provides a baseline for interpreting more elaborate charge-transfer patterns [8]. Such maps are particularly valuable for rationalizing the behavior of superatoms, doped materials, adsorption models, and charge-transfer systems [9]. The purpose of such a reference is not to replace high-precision experimental ionization potentials and electron affinities, or high-level wavefunction calculations for individual atoms, but to provide a transparent and internally consistent descriptor framework that can be transferred to larger systems where conceptual DFT descriptors are commonly evaluated at the DFT level.

This distinction is especially important for electron affinities. Atomic electron affinities are more sensitive than ionization potentials to basis-set quality, diffuse functions, self-interaction and delocalization errors, and the ability of the electronic-structure method to describe spatially extended excess-electron distributions. These issues become critical for weakly bound or unbound anions, for which a finite Gaussian basis may produce a localized SCF solution that should be interpreted as a diagnostic computational state rather than as a physical bound anion [10]. Therefore, a periodic donor–acceptor map based on electron-affinity-derived descriptors must be accompanied by both reference-data benchmarking and an explicit classification of the physical status of the anionic states.

In this work, we construct a periodic donor–acceptor descriptor map for main-group atoms from H to Kr using  $\Delta$ SCF-DFT calculations. Neutral atoms, monocations, and formally defined monoanionic states were computed to obtain ionization potentials and electron affinities, which were then used to derive conceptual DFT descriptors, including  $\chi$ ,  $\eta$ ,  $\mu$ ,  $\omega$ ,  $\omega^-$ , and  $\omega^+$ . The production dataset was obtained at the  $\omega$ B97X-D4/def2-QZVPPD level of theory and benchmarked against reference atomic data. Additional calculations using  $\omega$ B97X-D4/def2-TZVPPD, PBE0/def2-QZVPPD, and PBE0/def2-TZVPPD were performed to assess functional and basis-set sensitivity. Finally, the resulting descriptors were used to build donor–acceptor maps based on normalized  $D_{\text{rel}}$  and  $A_{\text{rel}}$  indices, defined so that larger values represent stronger relative donor and acceptor character, respectively.

This work extends previous atomic electrodonating/electroaccepting analyses by combining reference-data benchmarking, functional/basis-set sensitivity, normalized donor–acceptor mapping, and explicit classification of core, borderline, and diagnostic anionic cases. The resulting dataset offers a compact reference for interpreting atomic donor–acceptor behavior and for connecting isolated-atom descriptors with more complex systems such as clusters, superatoms, doped materials, and charge-transfer models. The separation between validated electron-affinity cases and finite-basis diagnostic anionic states is intended to prevent the overinterpretation of formally computed monoanions while preserving their value as methodological stress tests.

## 2. Computational Details

### 2.1. Atomic Dataset

The atomic dataset was composed of main-group elements from H to Kr, including H, He, Li–Ne, Na–Ar, K, Ca, and the p-block elements Ga–Kr. Transition metals were not included in order to avoid additional complications associated with dense manifolds of low-lying electronic states, multiple competing spin states, stronger scalar-relativistic and core-valence effects, stronger non-dynamical correlation and possible multireference character, and a higher risk of converging to electronically inconsistent or variationally collapsed SCF solutions in an automated  $\Delta$ SCF workflow. For each atom X, three electronic states were considered: the neutral atom X, the corresponding monocation  $X^+$ , and the formally defined monoanionic state  $X^-$ . This design allowed the direct evaluation of ionization potentials, electron affinities, and conceptual DFT descriptors using a  $\Delta$ SCF approach.

For each species, the charge and spin multiplicity were assigned according to the expected ground-state electron configuration. The  $H^+$  cation was treated as a special zero-electron reference, with an energy of 0.00  $E_h$ , rather than as a conventional SCF calculation. The complete list of atoms, charges, multiplicities, and input files is provided in the Supporting Information.

For open-shell calculations, the spin expectation value  $\langle S^2 \rangle$  reported by ORCA was compared with the ideal value  $S(S + 1)$  expected from the assigned spin multiplicity. The resulting  $\Delta\langle S^2 \rangle$  values were used as diagnostics for spin contamination. The full atom-by-atom spin diagnostics for the production and sensitivity calculations are provided in the Supporting Information as Tables S10a and S10b.

### 2.2. Quantum-Chemical Calculations

All calculations were performed with ORCA 6.0.1 [11,12]. ORCA input files were prepared using simple-input keyword lines and explicit Cartesian coordinates, with each atom placed at the origin. The NOCOSX keyword was used to avoid the chain-of-spheres approximation for exact exchange in these single-atom benchmark calculations. Since each job contained only one atom, the additional computational cost was negligible. A dense numerical grid was used through DefGrid3, and the SCF convergence was tightened with VeryTightSCF. A maximum of 500 SCF iterations was allowed.

The production calculations were carried out at the  $\omega$ B97X-D4/def2-QZVPPD level of theory, using the  $\omega$ B97X-D4 functional variant together with a diffuse property-optimized quadruple-zeta def2 basis set [13–16]. For isolated atoms, the atom–atom dispersion correction should not be interpreted as a physically important stabilization term because no interatomic dispersion pairs are present. The use of the D4-labeled functional is therefore retained as part of a consistent named functional protocol, whereas the aspects expected to be most relevant for the present atomic IP and EA calculations are the range-separated hybrid exchange treatment and the diffuse quadruple-zeta basis. The range-separated hybrid character of the  $\omega$ B97X family is appropriate for reducing delocalization-related errors in charged systems, while the def2-QZVPPD basis provides a diffuse quadruple-zeta description needed for weakly bound anionic states.

All calculations were performed with the standard nonrelativistic Hamiltonian associated with the selected all-electron def2 basis sets for the H–Kr range. Scalar-relativistic and explicit core–valence correlation effects were not included in the production protocol. This choice is consistent with the descriptor-map objective of the study, but fourth-period post-*d* atoms should be interpreted with additional caution because their IP and EA values can be more sensitive to scalar-relativistic and core–valence effects than those of lighter main-group atoms.

For the method-sensitivity analysis, three additional levels of theory were evaluated:  $\omega$ B97X-D4/def2-TZVPPD, to isolate the basis-set effect relative to the production method; PBE0/def2-QZVPPD, to evaluate functional sensitivity at the production basis-set level; and PBE0/def2-TZVPPD, to complete a compact  $2 \times 2$  functional/basis-set comparison [17,18]. Together with the production dataset, these levels provide a direct comparison between a range-separated hybrid and a global hybrid functional, as well as between diffuse triple-zeta and diffuse quadruple-zeta basis sets. The original def2 basis family was developed as a balanced set of split-valence, triple-zeta, and quadruple-zeta basis sets for broad periodic coverage, while the diffuse property-optimized extensions were developed to improve the description of response properties and diffuse electronic distributions. This compact  $2 \times 2$  design was chosen to isolate functional and diffuse basis-set effects without turning the study into an exhaustive functional benchmark; therefore, pure GGA and double-hybrid functionals were not included, and the comparison was restricted to chemically distinct hybrid DFT levels directly relevant to the production protocol.

### 2.3. Extraction of Ionization Potentials and Electron Affinities

Atomic ionization potentials and electron affinities were obtained from total electronic energies using a  $\Delta$ SCF scheme. For isolated atoms, the usual distinction between vertical and adiabatic values associated with nuclear-coordinate relaxation is not applicable, so the calculated energy differences correspond directly to atomic IP and EA values. For each atom  $X$ , the ionization potential was computed as

$$IP = E(X^+) - E(X), \quad (1)$$

and the electron affinity was computed as

$$EA = E(X) - E(X^-), \quad (2)$$

where all energies are electronic energies in hartree and the final values were converted to electronvolts.

By convention, a positive EA corresponds to a bound anion. Electron affinities were interpreted cautiously for diagnostic cases because NIST CCCBDB explicitly warns that electron-affinity calculations are strongly basis-set dependent and that many species have anions that are not bound relative to the neutral species plus a free electron.

### 2.4. Physical Interpretation of Diagnostic Anionic States

For atoms with experimentally bound ground-state monoanions, the  $\Delta$ SCF electron affinity can be interpreted as an approximation to the physical electron affinity, subject to the usual limitations of the electronic-structure method. However, this interpretation does not apply in the same way to atoms whose ground-state monoanions are not physically bound. In such cases, a finite localized Gaussian basis set may yield a formally converged anionic SCF solution with a negative  $\Delta$ SCF electron affinity. These values should not be interpreted as electron affinities of stable localized atomic anions. Instead, they are reported here as finite-basis diagnostic quantities that probe the behavior of the computational protocol when an excess electron is forced into a localized one-electron basis.

This distinction is important for noble gases and selected alkaline-earth or half-filled-shell atoms, for which stable ground-state monoanions are not generally formed [19,20]. In the complete-basis physical limit, an unbound excess electron is expected to detach to infinity, and the appropriate physical description is the neutral atom plus a free electron rather than a stable ground-state monoanion. Therefore, diagnostic anionic cases are retained only to document the numerical behavior of the  $\Delta$ SCF workflow and to delimit the

scope of the resulting donor–acceptor descriptors. They are not used as ordinary bound-anion validation cases and should not be assigned the same quantitative interpretation as atoms with experimentally established positive electron affinities.

### 2.5. Conceptual DFT Descriptors

Conceptual DFT descriptors were calculated from the  $\Delta$ SCF ionization potentials and electron affinities. The electronegativity  $\chi$ , chemical hardness  $\eta$ , and electronic chemical potential  $\mu$  were obtained as

$$\chi = \frac{IP + EA}{2}, \quad (3)$$

$$\eta = \frac{IP - EA}{2}, \quad (4)$$

$$\mu = -\chi. \quad (5)$$

The global electrophilicity index was calculated as

$$\omega = \frac{\mu^2}{2\eta}, \quad (6)$$

following the electrophilicity framework introduced by Parr, von Szentpály, and Liu.

The electrodonating and electroaccepting powers were calculated using the finite-difference expressions introduced by Gázquez, Cedillo, and Vela [6]. In that formulation, separate left- and right-side parabolic approximations to the energy as a function of electron number lead to effective chemical potentials  $\mu^- = -(3IP + EA)/4$  and  $\mu^+ = -(IP + 3EA)/4$ , together with  $\eta = (IP - EA)/2$ . Substitution into the corresponding electrophilicity-like expressions gives

$$\omega^- = \frac{(3IP + EA)^2}{16(IP - EA)}, \quad (7)$$

$$\omega^+ = \frac{(IP + 3EA)^2}{16(IP - EA)}, \quad (8)$$

The factor 16 in the denominator, therefore, follows directly from the squared one-quarter factors in  $\mu^-$  and  $\mu^+$ , combined with  $\eta = (IP - EA)/2$ , and is part of the original Gázquez–Cedillo–Vela definition. In this convention,  $\omega^-$  measures the resistance to electron donation, so smaller  $\omega^-$  values correspond to stronger electron-donating ability, whereas larger  $\omega^+$  values correspond to stronger electron-accepting ability. To facilitate periodic comparison, relative donor and acceptor indices were constructed using Na and F as reference atoms, respectively:

$$D_{\text{rel}}(X) = \frac{\omega_{\text{Na}}^-}{\omega_X^-}, \quad (9)$$

$$A_{\text{rel}}(X) = \frac{\omega_X^+}{\omega_{\text{F}}^+}. \quad (10)$$

Thus, Na has  $D_{\text{rel}} = 1$  and F has  $A_{\text{rel}} = 1$ . The donor index was defined as an inverse relative  $\omega^-$  ratio so that larger  $D_{\text{rel}}$  values indicate stronger relative donor character, whereas  $A_{\text{rel}}$  was defined directly from  $\omega^+$  so that larger  $A_{\text{rel}}$  values indicate stronger relative acceptor character.

### 2.6. Reference Data and Validation

Reference ionization potentials were obtained from the NIST Atomic Spectra Database (NIST ASD) [21], which provides critically evaluated ground-state and ionization-energy

data for atoms and atomic ions. Electron-affinity reference values were updated using recent peer-reviewed compilations of recommended atomic electron affinities. The primary source was the review by Ning and Lu, which summarizes recommended electron affinities and energy levels of atomic negative ions across the periodic table. The updated review by Yan, Lu, Zhang, and Ning was additionally used for the most recent arsenic value and for cross-checking the recommended main-group electron-affinity dataset. The NIST Chemistry WebBook and CCCBDB entries [22,23] were retained only as secondary database cross-checks rather than as the primary electron-affinity reference source.

The validation was divided into three categories. First, atoms with well-established positive electron affinities were used as the main quantitative EA validation set. Second, Ca was retained as a weak or borderline EA validation case because its experimental electron affinity is very small, and the computed values are sensitive to the functional and basis set. Third, He, Be, N, Ne, Mg, Ar, and Kr were treated as diagnostic cases for electron-affinity-derived descriptors because their ground-state monoanions are not physically bound in the same sense as the core validation set, or because no directly comparable positive experimental electron affinity is available for quantitative validation.

The reference uncertainties associated with the IP and EA values were retained in the validation dataset and are reported in the Supporting Information. These uncertainties are substantially smaller than the corresponding DFT deviations for the present benchmark and therefore do not affect the qualitative assessment of method performance.

The accuracy of each method was quantified using the mean error (ME), mean absolute error (MAE), and root mean square error (RMSE):

$$ME = \frac{1}{n} \sum_{i=1}^n (P_i^{\text{calc}} - P_i^{\text{ref}}), \quad (11)$$

$$MAE = \frac{1}{n} \sum_{i=1}^n |P_i^{\text{calc}} - P_i^{\text{ref}}|, \quad (12)$$

$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^n (P_i^{\text{calc}} - P_i^{\text{ref}})^2}. \quad (13)$$

Here,  $P$  corresponds to either IP or EA. The MAE was used as the primary measure of average accuracy, while the RMSE was used to identify whether the error distribution was affected by large outliers.

## 2.7. Quality Control and Data Extraction

All ORCA output files were checked for successful completion using the normal termination message. The final production and sensitivity datasets contained 77 energy entries and 26 descriptor rows each. All extracted data were processed using Python 3.14 scripts to calculate IP, EA, conceptual DFT descriptors, validation errors, and normalized donor–acceptor indices. The corresponding input files, extracted energy tables, descriptor tables, validation data, and processing scripts are provided in the Supporting Information to ensure full reproducibility.

## 2.8. Use of Generative Artificial Intelligence Tools

During the preparation of this manuscript and its Supplementary Materials, ChatGPT (GPT-5.4) was used as an AI-assisted tool to support language editing, LaTeX formatting assistance, editorial revision, and the preparation of supplementary files. Quantum-chemical calculations were performed with ORCA 6.0.1, and all numerical values reported in the manuscript were derived from the corresponding ORCA calculation outputs and extracted data files. No GenAI tool was used to perform the quantum-chemical calculations or

to autonomously generate, alter, validate, or interpret the numerical data. The author reviewed, edited, and verified all AI-assisted outputs and takes full responsibility for the content of this publication.

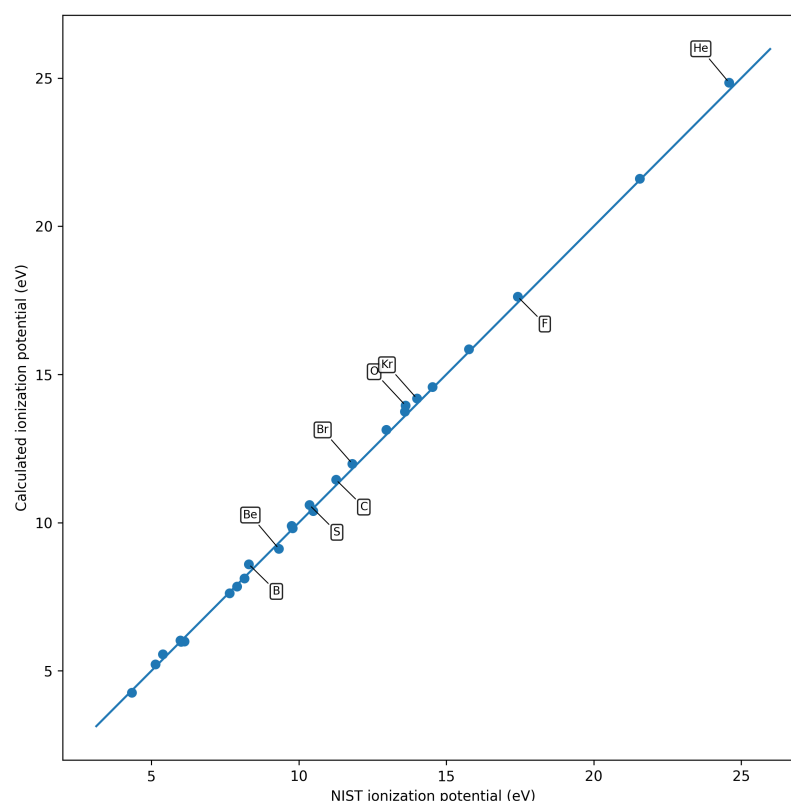
### 3. Results and Discussion

#### 3.1. Accuracy of the Production Level of Theory

The first objective of this work was to determine whether a single production level of theory could reproduce the reference atomic ionization potentials and electron affinities with sufficient accuracy to support a donor–acceptor descriptor analysis. The  $\omega$ B97X-D4/def2-QZVPPD level was selected as the production method because it combines a range-separated hybrid functional with a diffuse quadruple-zeta basis set, a combination expected to be especially relevant for anionic states and electron-affinity calculations.

For the complete set of 26 main-group atoms from H to Kr, the production method gives an ionization-potential mean absolute error (MAE) of 0.134 eV and a root mean square error (RMSE) of 0.161 eV. The corresponding mean signed error is 0.087 eV, indicating a mild tendency to overestimate the ionization potentials. The largest absolute deviation is observed for O (0.338 eV), but even this value remains small for a compact atom-by-atom benchmark spanning a broad range of first ionization energies.

The parity plot in Figure 1 confirms this behavior visually. Most atoms lie close to the ideal diagonal, and the deviations do not display a strong systematic drift across the full energy range. This result is important because the ionization potential enters directly into the conceptual DFT descriptors used below; therefore, errors in IP would propagate into the hardness, chemical potential, electrophilicity, and donor/acceptor powers.



**Figure 1.** Parity plot comparing calculated and NIST ionization potentials for the production method. Only the atoms with the largest deviations from the diagonal are labeled to avoid visual crowding.

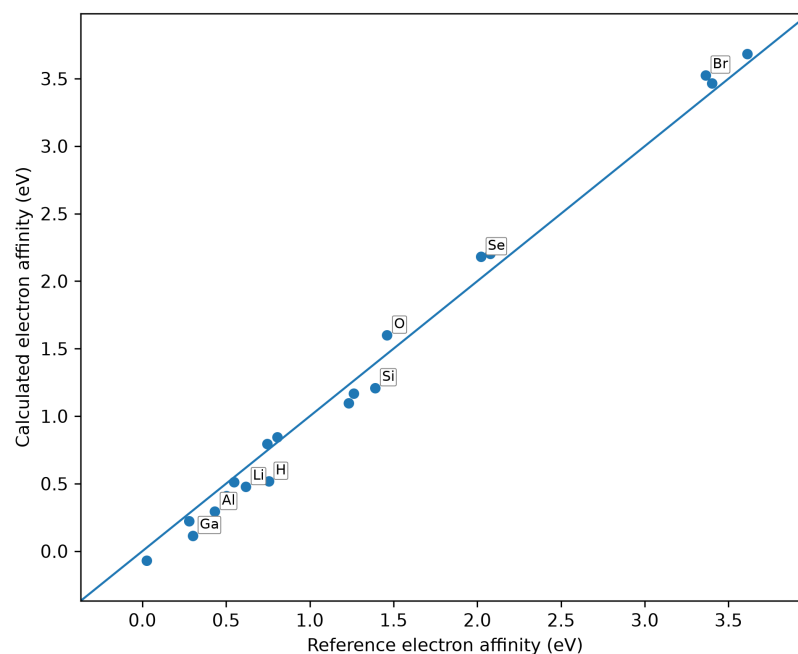
The electron-affinity validation is more demanding because it requires an accurate description of neutral and anionic atomic states. For the 19 atoms with reference EA values

included in the validation set, the production method gives an EA MAE of 0.116 eV and an RMSE of 0.128 eV when the weak calcium affinity is retained. Excluding Ca changes the EA MAE to 0.117 eV and the RMSE to 0.130 eV, showing that the overall validation is not dominated by this borderline case.

This behavior is consistent with previous reviews of atomic and molecular electron affinities, which emphasize that EA values are generally more sensitive than ionization potentials to basis-set completeness, diffuse functions, and the ability of the electronic-structure method to describe spatially extended excess-electron distributions. Rienstra-Kiracofe and co-workers highlighted that both experimental and theoretical electron affinities require special care, particularly when the anionic state is weakly bound or close to the detachment threshold [10]. Therefore, the larger relative difficulty observed for EA compared with IP in the present benchmark is not unexpected, but rather reflects a known limitation of anion-sensitive calculations.

Figure 2 shows that the production method also follows the reference EA trend with acceptable accuracy. The largest residuals are associated with atoms whose electron affinities are comparatively small or whose anions are known to be delicate from a computational standpoint. This is consistent with the expected greater basis-set and functional sensitivity of electron affinities relative to ionization potentials.

The reference uncertainties are not shown as error bars in Figures 1 and 2 because they are smaller than the plotted symbols on the scale of the figures. For the production dataset, the median reference uncertainty is  $3 \times 10^{-6}$  eV for IP values and  $6 \times 10^{-6}$  eV for validated EA values, whereas the median absolute DFT deviations are 0.126 eV for IP and 0.127 eV for EA. The full uncertainty table is provided in the Supporting Information as Table S8a,b.



**Figure 2.** Parity plot comparing calculated and reference electron affinities for the production method. Labeled atoms correspond to the largest deviations from the diagonal.

Table 1 serves two purposes. First, it provides the atom-by-atom validation of the production method against reference atomic data. Ionization-potential reference values were taken from NIST ASD, whereas electron-affinity reference values were taken from the updated peer-reviewed compilations described above. Second, the table defines the interpretation class used throughout the rest of the manuscript. The core validation atoms are those for which both IP and EA values are available and chemically meaningful for

quantitative comparison. In contrast, He, Be, N, Ne, Mg, Ar, and Kr were retained as diagnostic cases because their ground-state monoanions are not physically bound in the same sense as the core validation set. This distinction is essential because formally computed anionic energies can still be useful for testing the numerical behavior of the method, but they should not be assigned the same interpretive weight as validated EA-derived descriptors.

Spin contamination was also inspected for the unrestricted open-shell calculations. In the production dataset, all reported  $\langle S^2 \rangle$  values were close to the ideal  $S(S+1)$  values, with a maximum absolute deviation of 0.023. Across all four tested method–basis combinations, no calculation exceeded  $|\Delta\langle S^2 \rangle| = 0.05$ . Therefore, the observed IP and EA deviations are not attributable to substantial spin contamination in the unrestricted atomic calculations.

**Table 1.** Production-level ionization potentials, electron affinities, and validation classes.

| Element | IP Ref.<br>(eV) | IP Calc.<br>(eV) | IP Error<br>(eV) | EA Ref.<br>(eV) | EA Calc.<br>(eV) | EA Error<br>(eV) | EA Validation Class           |
|---------|-----------------|------------------|------------------|-----------------|------------------|------------------|-------------------------------|
| H       | 13.598          | 13.750           | 0.151            | 0.754           | 0.517            | −0.237           | core                          |
| He      | 24.587          | 24.853           | 0.265            | –               | −8.049           | –                | diagnostic/not bound          |
| Li      | 5.392           | 5.564            | 0.172            | 0.618           | 0.478            | −0.140           | core                          |
| Be      | 9.323           | 9.120            | −0.203           | –               | −0.537           | –                | diagnostic/not bound          |
| B       | 8.298           | 8.602            | 0.304            | 0.280           | 0.222            | −0.058           | core                          |
| C       | 11.260          | 11.448           | 0.188            | 1.262           | 1.169            | −0.093           | core                          |
| N       | 14.534          | 14.582           | 0.048            | –               | −0.207           | –                | diagnostic/not bound          |
| O       | 13.618          | 13.956           | 0.338            | 1.461           | 1.599            | 0.138            | core                          |
| F       | 17.423          | 17.624           | 0.201            | 3.401           | 3.465            | 0.063            | core                          |
| Ne      | 21.565          | 21.613           | 0.048            | –               | −2.021           | –                | diagnostic/not bound          |
| Na      | 5.139           | 5.225            | 0.086            | 0.548           | 0.513            | −0.035           | core                          |
| Mg      | 7.646           | 7.617            | −0.029           | –               | −0.432           | –                | diagnostic/not bound          |
| Al      | 5.986           | 6.033            | 0.047            | 0.433           | 0.293            | −0.140           | core                          |
| Si      | 8.152           | 8.120            | −0.032           | 1.390           | 1.210            | −0.180           | core                          |
| P       | 10.487          | 10.397           | −0.089           | 0.747           | 0.794            | 0.048            | core                          |
| S       | 10.360          | 10.597           | 0.237            | 2.077           | 2.204            | 0.127            | core                          |
| Cl      | 12.968          | 13.131           | 0.163            | 3.613           | 3.683            | 0.070            | core                          |
| Ar      | 15.760          | 15.849           | 0.089            | –               | −1.203           | –                | diagnostic/not bound          |
| K       | 4.341           | 4.261            | −0.079           | 0.501           | 0.410            | −0.092           | core                          |
| Ca      | 6.113           | 6.000            | −0.113           | 0.025           | −0.068           | −0.093           | weak/borderline EA validation |
| Ga      | 5.999           | 5.982            | −0.018           | 0.301           | 0.115            | −0.186           | core                          |
| Ge      | 7.899           | 7.845            | −0.055           | 1.233           | 1.095            | −0.138           | core                          |
| As      | 9.789           | 9.810            | 0.022            | 0.804           | 0.844            | 0.040            | core                          |
| Se      | 9.752           | 9.892            | 0.139            | 2.021           | 2.180            | 0.159            | core                          |
| Br      | 11.814          | 11.992           | 0.178            | 3.364           | 3.526            | 0.162            | core                          |
| Kr      | 14.000          | 14.191           | 0.191            | –               | −1.141           | –                | diagnostic/not bound          |

The signed errors in Table 1 also reveal that the production method does not introduce a uniform systematic bias across the periodic series. For IP values, both positive and negative deviations are present, although the overall mean signed error remains positive. For EA values, the largest deviations occur for atoms with relatively small or delicate electron affinities, such as Ga and Ca. The Ga residual should be interpreted cautiously because Ga is a fourth-period post-*d* element with a filled 3*d* shell, making it potentially more sensitive to scalar-relativistic and core–valence effects than lighter main-group atoms [24]. Similar, although less pronounced, considerations apply to the neighboring fourth-period main-group elements. These effects are outside the present production protocol and represent a limitation of the nonrelativistic descriptor map rather than a failure of the donor–acceptor classification itself.

### 3.2. Functional and Basis-Set Sensitivity

The second objective was to test whether the descriptor trends obtained at the production level are robust with respect to the functional and the basis set. To this end, the production calculation was compared with three additional combinations:  $\omega$ B97X-D4/def2-TZVPPD, PBE0/def2-QZVPPD, and PBE0/def2-TZVPPD. Together, these calculations form a compact two-by-two sensitivity matrix that separates functional effects from basis-set effects.

The ionization potentials are comparatively insensitive to the basis-set change. With  $\omega$ B97X-D4, replacing def2-QZVPPD by def2-TZVPPD changes the IP MAE only from 0.134 to 0.136 eV. PBE0 gives slightly smaller IP MAEs, 0.116 eV with def2-QZVPPD and 0.112 eV with def2-TZVPPD, indicating that the first ionization potentials are relatively robust for the tested hybrid and range-separated hybrid functionals.

The behavior is different for electron affinities. At fixed  $\omega$ B97X-D4, reducing the basis from def2-QZVPPD to def2-TZVPPD increases the EA MAE from 0.116 to 0.219 eV and the EA RMSE from 0.128 to 0.257 eV when Ca is retained. The same basis-set sensitivity is evident for PBE0, for which the EA MAE increases from 0.136 eV with def2-QZVPPD to 0.257 eV with def2-TZVPPD, while the corresponding RMSE increases from 0.266 to 0.422 eV. This result provides direct evidence that the diffuse quadruple-zeta basis is not merely a conservative choice, but an important requirement for stable treatment of atomic anions in this dataset.

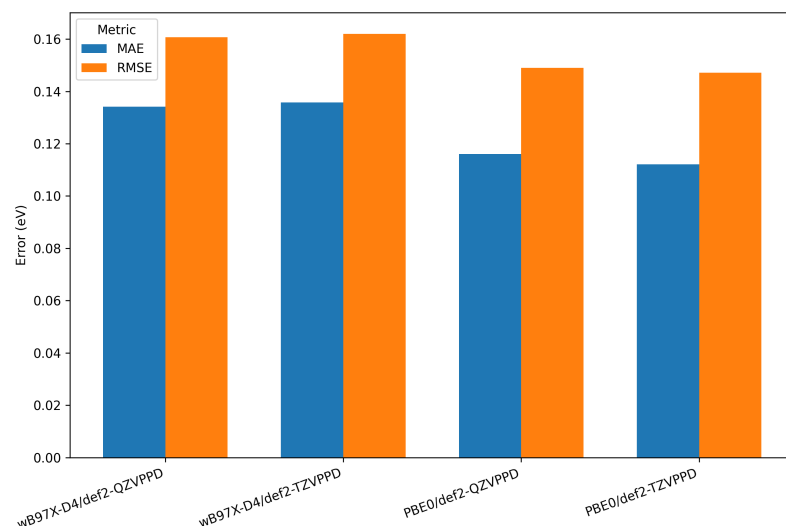
This conclusion is consistent with the design purpose of diffuse property-optimized basis sets. The def2 basis family was developed to provide balanced basis-set quality across the periodic table, while the property-optimized diffuse extensions were introduced to improve the description of response properties and diffuse electronic distributions [15,16]. Such diffuse flexibility is especially important for anions, where the excess electron may occupy a spatially extended orbital. The present sensitivity analysis therefore provides a direct atom-by-atom demonstration of the same principle: IP values are relatively stable with respect to the triple-zeta/quadruple-zeta change, whereas EA values respond much more strongly to the quality of the diffuse basis. The numerical impact of these functional and basis-set changes is summarized in Table 2 and visualized in Figures 3 and 4.

**Table 2.** Summary error metrics for the four tested method–basis combinations.

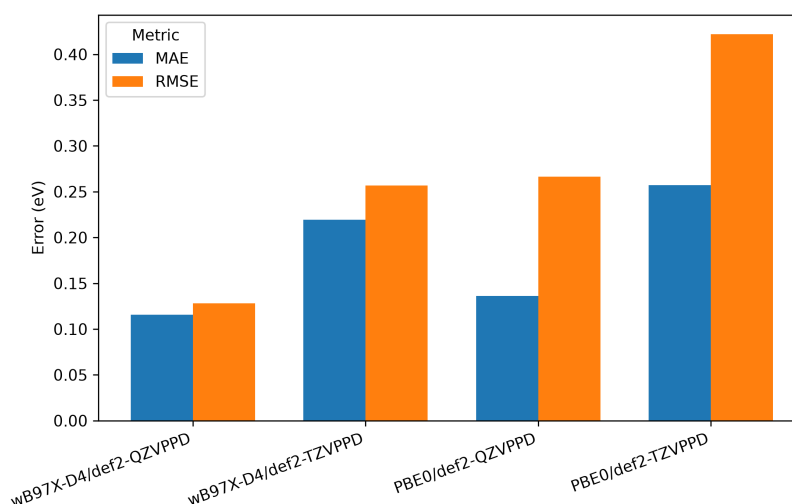
| Method                       | IP MAE (eV) | IP RMSE (eV) | EA MAE Incl. Ca (eV) | EA RMSE Incl. Ca (eV) | EA MAE Excl. Ca (eV) | EA RMSE Excl. Ca (eV) |
|------------------------------|-------------|--------------|----------------------|-----------------------|----------------------|-----------------------|
| $\omega$ B97X-D4/def2-QZVPPD | 0.134       | 0.161        | 0.116                | 0.128                 | 0.117                | 0.130                 |
| $\omega$ B97X-D4/def2-TZVPPD | 0.136       | 0.162        | 0.219                | 0.257                 | 0.221                | 0.259                 |
| PBE0/def2-QZVPPD             | 0.116       | 0.149        | 0.136                | 0.266                 | 0.088                | 0.139                 |
| PBE0/def2-TZVPPD             | 0.112       | 0.147        | 0.257                | 0.422                 | 0.191                | 0.269                 |

Thus, the bar plots emphasize the central conclusion of the sensitivity analysis: IP errors remain relatively stable across the tested levels, whereas EA errors increase markedly when the basis is reduced from def2-QZVPPD to def2-TZVPPD.

The comparison also clarifies the role of the functional. PBE0/def2-QZVPPD provides the lowest IP MAE and performs well for the core EA set when Ca is excluded, but it shows a larger RMSE when Ca is retained because the weak calcium electron affinity is difficult to reproduce. Conversely,  $\omega$ B97X-D4/def2-QZVPPD provides a more balanced behavior across both IP and EA metrics. For this reason, the production descriptor maps discussed below are based on  $\omega$ B97X-D4/def2-QZVPPD, while the PBE0 results are used as a methodological consistency check.



**Figure 3.** Mean absolute error and root mean square error for the ionization potentials obtained with the four tested methods.



**Figure 4.** Mean absolute error and root mean square error for electron affinities obtained with the four tested method–basis combinations. Metrics include Ca as a weak/borderline EA validation case.

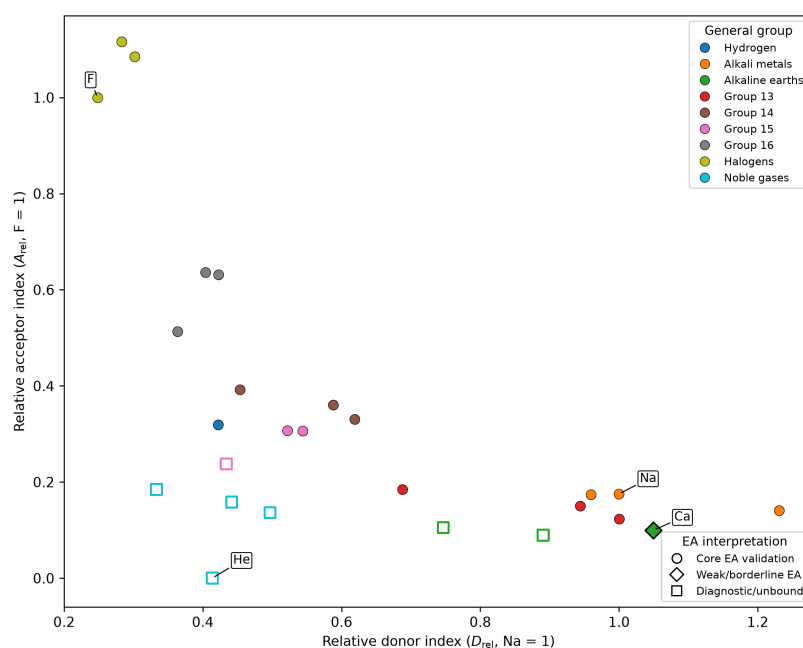
The contrast between PBE0 and  $\omega$ B97X-D4 should be interpreted primarily as a comparison between a global hybrid functional and a range-separated hybrid functional within the same  $\Delta$ SCF framework. Although the production method carries the D4 label, dispersion is not expected to be a relevant physical contribution for isolated atoms because there are no interatomic dispersion contacts. Thus, the improved balance of the production protocol should not be attributed to dispersion stabilization, but rather to the combined effect of the range-separated hybrid functional form and the diffuse quadruple-zeta basis used to describe neutral, cationic, and anionic atomic states.

### 3.3. Donor–Acceptor Descriptor Map

The production-level IP and EA values were transformed into conceptual DFT descriptors, including electronegativity, hardness, chemical potential, electrophilicity, electron-donating power, and electron-accepting power. The donor and acceptor powers were then normalized using Na and F as reference atoms, respectively. This normalization gives a compact descriptor map in which values near unity represent behavior comparable to the reference donor or acceptor.

The observed map is also consistent with the conceptual meaning of the Gázquez–Cedillo–Vela descriptors. In that framework, smaller  $\omega^-$  values correspond to greater electron-donating ability, whereas larger  $\omega^+$  values correspond to stronger electron-accepting behavior [6]. The normalized donor index used here was therefore defined as the inverse relative  $\omega^-$  ratio with respect to Na, so that larger  $D_{\text{rel}}$  values can be read directly as stronger donor character. This convention preserves the physical interpretation of  $\omega^-$  while making the donor axis visually intuitive.

The resulting donor–acceptor map is shown in Figure 5. Points are colored by general periodic-table group, while the marker style distinguishes the physical interpretation class of the electron-affinity-derived descriptors. Filled circles correspond to core EA validation atoms, the diamond identifies Ca as a weak/borderline EA case, and open squares indicate diagnostic finite-basis anionic cases. This representation preserves the periodic trends while preventing diagnostic anionic states from being visually conflated with validated bound-anion descriptors.



**Figure 5.** Donor–acceptor map obtained from the production-level descriptors. Points are colored by general periodic-table group. Filled circles indicate atoms in the core electron-affinity validation set, the diamond marks Ca as a weak/borderline electron-affinity case, and open squares indicate diagnostic finite-basis anionic cases. Diagnostic cases are shown to document the behavior of the formal descriptor equations but should not be interpreted as validated descriptors of stable bound atomic anions.

The donor axis reproduces the expected electropositive trend. The strongest donor region is occupied by K (1.231), Ca (1.050), Ga (1.000), and Na by definition (1.000). The halogens occupy the opposite side of the donor axis, with F (0.248), Cl (0.283), and Br (0.302) showing much lower relative donor indices.

The acceptor axis follows the complementary trend. Halogens are the strongest acceptors, with Cl (1.116), Br (1.085), and F by definition (1.000) defining the high-acceptor region. Chalcogens such as S (0.636) and Se (0.632) also show elevated acceptor character, whereas He, Mg, Ca, Be, and Ga define the weak-acceptor region. This distribution is chemically intuitive and supports the use of the normalized map as a compact tool for periodic descriptor analysis.

The quantitative interpretation of these trends is restricted to the core validation atoms and the explicitly marked weak/borderline case; diagnostic points are included only to show the formal behavior of the descriptor equations.

These trends are in line with the atomic periodic behavior reported by Orozco-Valencia and Vela, who evaluated electrodonating and electroaccepting powers for neutral atoms and used them to rationalize the distribution of atoms in the electrodonating–electroaccepting plane [25]. Their analysis supports the idea that the  $\omega^-/\omega^+$  framework can capture periodic donor–acceptor trends, while the present work extends that idea by combining  $\Delta$ SCF-DFT benchmarked against reference atomic data with explicit functional and basis-set sensitivity analysis.

### 3.4. Diagnostic and Borderline Anions

A key point of the present study is that not all formally computed monoanions have the same physical status. Several atoms, including He, Be, N, Ne, Mg, Ar, and Kr, were retained as diagnostic cases because their ground-state monoanions are not experimentally established as stable bound anions in the same sense as the core validation set. The broader atomic electron-affinity literature reports that Be and Mg do not form stable ground-state negative ions, that N does not form a stable negative ion, and that noble-gas atoms do not form stable ground-state negative ions, although selected metastable anionic states may exist for some elements [19,20]. Therefore, the negative  $\Delta$ SCF electron affinities obtained for these atoms should be interpreted as finite-basis diagnostic results, not as physical electron affinities of stable localized monoanions.

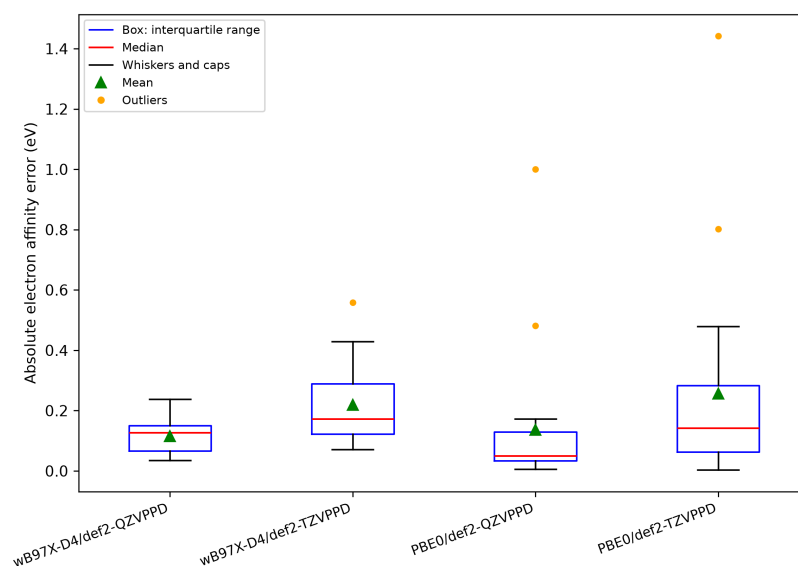
This distinction is particularly important because localized Gaussian basis sets can artificially confine an excess electron that would otherwise detach in the complete-basis physical limit. The resulting SCF energies are mathematically well defined within the chosen finite basis, and they are useful for stress-testing the numerical behavior of the workflow, but they should not be assigned the same physical meaning as validated positive electron affinities. Consequently, descriptors derived from such diagnostic EA values are included only to show the behavior of the formal descriptor equations at the boundary of anion stability. They should be interpreted qualitatively and should not be used as quantitative descriptors of genuine bound atomic anions.

Calcium requires a separate discussion. Experimentally, Ca has a very small positive electron affinity, whereas all four tested method–basis combinations predict a slightly negative EA. In the production method, the absolute deviation is modest, but the sign inversion shows that Ca lies near the practical resolution limit of the tested DFT/basis-set combinations for weakly bound atomic anions. This behavior is consistent with the general sensitivity of weakly bound anions to basis-set completeness, diffuse functions, and the electronic-structure method [10,19]. Therefore, the negative calculated EA should not be interpreted as evidence that Ca lacks a physical bound anion, but rather as evidence that this weakly bound case is particularly sensitive to the approximate functional and basis set. For this reason, Ca is treated as a weak or borderline EA validation case rather than as either a conventional core validation atom or a purely diagnostic unbound-anion case.

The sensitivity analysis provides additional evidence for this interpretation. The list of atoms predicted to have negative electron affinities expands when the basis set is reduced to def2-TZVPPD. For example, Ga becomes negative with  $\omega$ B97X-D4/def2-TZVPPD, and H becomes negative with PBE0/def2-TZVPPD. These changes are not evidence for changes in the physical stability of the corresponding anions; rather, they reflect the delicate balance involved in describing weakly bound excess-electron states. They also reinforce the decision to use the diffuse quadruple-zeta basis for the production descriptor map.

### 3.5. Distribution of Electron-Affinity Errors

The distribution of absolute EA errors is summarized in Figure 6.



**Figure 6.** Distribution of absolute electron-affinity errors for the four tested method–basis combinations. Boxes show the interquartile range, red lines indicate medians, green triangles indicate means, and orange points indicate outliers.

This representation complements the MAE and RMSE values by showing whether the error is broadly distributed or dominated by a small number of outlying atoms. The production method combines a low central tendency with a comparatively controlled spread, whereas the triple-zeta calculations show broader EA-error distributions. This behavior is consistent with the larger RMSE values observed for the triple-zeta methods and further supports the use of  $\omega$ B97X-D4/def2-QZVPPD for the final donor–acceptor map.

### 3.6. Overall Assessment

Taken together, the results support the use of  $\omega$ B97X-D4/def2-QZVPPD as the production level for the construction of periodic donor–acceptor maps. The method gives accurate ionization potentials, acceptable electron affinities for the validated atoms, and a chemically meaningful distribution of normalized donor and acceptor indices. The sensitivity analysis shows that the ionization potentials are relatively stable with respect to the tested functional and basis-set changes, while the electron affinities are substantially more sensitive to the basis set. The final descriptor map should therefore be interpreted as a robust production-level representation for the validated atoms, with separate qualitative discussion reserved for diagnostic and borderline anionic cases.

## 4. Conclusions

This work presents a validated periodic donor–acceptor descriptor map for main-group atoms from H to Kr using a  $\Delta$ SCF-DFT framework. Neutral atoms, monocations, and formally defined monoanionic states were calculated to obtain ionization potentials and electron affinities, which were then used to derive conceptual DFT descriptors, including electronegativity, hardness, chemical potential, electrophilicity, electrodonating power, and electroaccepting power. By comparing the calculated values with reference atomic data, using NIST ASD for ionization potentials and updated recommended compilations for electron affinities, the study establishes a reproducible computational basis for interpreting atomic donor–acceptor behavior.

The production level,  $\omega$ B97X-D4/def2-QZVPPD, provided a balanced description of the properties required for the descriptor analysis. Ionization potentials were reproduced with low errors across the full atomic set, while electron affinities showed acceptable agreement for the validated atoms despite their known sensitivity to anionic-state description. The sensitivity analysis demonstrated that IP values are comparatively robust with respect to the tested functional and basis-set changes, whereas EA values are significantly more dependent on the quality of the diffuse basis set. In particular, the comparison between def2-QZVPPD and def2-TZVPPD confirmed that the diffuse quadruple-zeta basis is important for achieving stable and reliable electron-affinity trends.

The normalized donor–acceptor map obtained from the production descriptors reproduces chemically meaningful periodic behavior. Alkali metals occupy the strong-donor region, halogens define the strong-acceptor region, and intermediate main-group elements distribute according to their expected donor–acceptor character. The use of normalized  $D_{\text{rel}}$  and  $A_{\text{rel}}$  indices provides an intuitive representation in which larger values correspond to stronger relative donor and acceptor behavior, respectively. This makes the resulting map useful as a compact reference for interpreting atomic trends and for comparison with more complex systems such as clusters, superatoms, doped materials, and charge-transfer models.

A key outcome of the study is the explicit separation between core validation atoms, weak or borderline electron-affinity cases, and diagnostic anions. Atoms such as He, Be, N, Ne, Mg, Ar, and Kr were retained as diagnostic cases but should not be interpreted with the same quantitative weight as atoms with validated electron affinities. Calcium, in particular, illustrates the difficulty of weakly bound anions: although its experimental EA is slightly positive, all tested method–basis combinations predicted a slightly negative value. This does not invalidate the protocol, but it emphasizes the practical resolution limit of DFT-based EA calculations for borderline anionic states.

Overall, the results support  $\omega$ B97X-D4/def2-QZVPPD as a suitable production level for constructing nonrelativistic main-group atomic donor–acceptor descriptor maps. The dataset, input files, descriptor tables, validation data, and processing scripts provided in the Supporting Information are intended to make the analysis reproducible and reusable. Scalar-relativistic and explicit core–valence effects were not included in the production protocol and may require additional testing for more quantitative treatment of fourth-period post-*d* elements. Future extensions of this work may include heavier main-group elements, relativistic corrections, higher-level wavefunction benchmarks with basis-set extrapolation for weak electron affinities, alternative functionals specifically optimized for electron affinities, and applications of the atomic reference map to clusters, superatoms, and functionalized materials.

**Supplementary Materials:** The following supporting information can be downloaded at: <https://www.mdpi.com/article/10.3390/atoms14070048/s1>. The Supplementary Data package contains the Production and Sensitivity folders, ORCA input files, processing scripts, and machine-readable tables. The Production folder includes the production-level atomic dataset, extracted energies, conceptual DFT descriptors, donor–acceptor indices, IP and EA validation data, negative-EA flags, quality-control summaries, reference uncertainty data, classified donor–acceptor map data, and spin expectation diagnostics. The Sensitivity folder includes the corresponding method-comparison data for the tested functional and basis-set combinations, including energy summaries, descriptor tables, validation tables, method metrics, negative-EA flags, quality-control summaries, and spin-contamination diagnostics. The machine-readable tables include: Table S1, Atomic dataset charges and multiplicities; Table S2, Production energies; Table S3a, Production descriptors; Table S3b, Donor–acceptor indices; Table S4a, IP validation; Table S4b, EA validation; Table S5, Method metrics; Table S6, Negative EA flags; Table S7, QC summary; Table S8a, Reference uncertainties; Table S8b, Reference

uncertainty summary; Table S9, Classified donor–acceptor map data; Table S10a, Spin expectation diagnostics; Table S10b, Spin contamination summary.

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**Data Availability Statement:** The data supporting the findings of this study are available in the Supplementary Materials including ORCA input files, extracted energy tables, descriptor tables, validation data, reference uncertainty tables, spin diagnostics, classified donor–acceptor map data, and processing scripts.

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