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Editorial

Computational Insights into Industrial Chemistry

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Abstract: This brief Editorial is dedicated to announcing the Special Issue "Computational Insights into Industrial Chemistry". The Special Issue covers the most recent progress in the rapidly growing field of computational chemistry, and the application of computer modeling in topics relevant to industrial chemistry (chemical industrial processes and materials, environmental effects caused by chemical industry activities, computer-aided design of catalysts, green chemistry, etc.).

Keywords: computational chemistry; computer modeling; industrial chemistry

One of the most important challenges for modern industrial chemistry is creation of smart technologies allowing to rational design of promising processes and materials to improve sustainability. Computer modeling (including quantum chemistry (ab initio and DFT), molecular dynamics simulation, machine learning in chemistry, computational biochemistry, cheminformatics, etc.) could provide a solid theoretical background for understanding the environmental effects caused by chemical industry activities on a molecular level. In particular, important theoretical methods in this regard are: topological analysis of the electron density distribution within the framework of Bader's theory (QTAIM) [1]; investigation of different effects of crystal packing using Hirshfeld surface analysis [2]; analysis of natural bond orbitals; and charges within the framework of Weinhold theory (NBO) [3]. It is possible to calculate the molecular surface electrostatic potential for the identification of areas most susceptible to nucleophilic, electrophilic, and radical attacks or analyze for these purposes the Fukui functions based on the frontier molecular orbitals [4]. The theoretical estimation of the adiabatic and vertical dissociation energies of supramolecular ensembles and the subsequent correction of these energies considering the basis set superposition error according to the Boys–Bernardi technique (BSSE correction) [5] can provide us with some ideas about the stability of materials and catalysts. The theoretical calculation of thermochemical parameters for model supramolecular association/dissociation processes—in particular, the enthalpy and Gibbs free energy of formation—helps us to understand the thermodynamics of self-organization. Application of theoretical model of the principle of hard and soft acids and bases (HSAB principle theoretical model) is very promising in the search for various correlations between theoretically calculated (e.g., chemical potential, hardness and softness, global indices of electrophilicity, and nucleophilicity) and experimentally observed (e.g., spectral characteristics, conductivity, magnetic and photo-physical properties) parameters, which could be useful for planning the manufacture of devices for pharmacology and biotechnology. Research in the field of computational chemistry can shed light on the relative stability of various inorganic, organic, organometallic and coordination compounds, which can act as building blocks for the creation of smart materials, their structural features, UV-Vis, IR, Raman and NMR spectral characteristics, conformational transitions and rotation barriers of functional groups. Finally, molecular dynamics [6], molecular mechanics [7], and Monte Carlo simulations [8] can provide us with important information regarding the solvation processes involving different chemical compound relevant for industrial chemistry.

Thus, the computer-aided molecular design of new materials or catalysts is a cutting-edge topic for industrial chemistry, and this Special Issue of *Computation* (belonging to the section "Computational Chemistry") is open for contributions from both junior and senior researchers from chemistry, physics, mathematics, informational technology, biology, ecology, and other related disciplines. All types of papers (reviews, mini-reviews, full papers, short communications, and technical notes, highlights, etc.) are welcome for consideration.

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References

1. Bader, R.F.W. A Quantum-Theory of Molecular-Structure and Its Applications. *Chem. Rev.* **1991**, *91*, 893–928. [CrossRef]
2. Spackman, M.A.; Jayatilaka, D. Hirshfeld Surface Analysis. *CrystEngComm* **2009**, *11*, 19–32. [CrossRef]
3. Glendening, E.D.; Landis, C.R.; Weinhold, F. Natural Bond Orbital Methods. *Wiley Interdiscip. Rev. Comput. Mol. Sci.* **2012**, *2*, 1–42. [CrossRef]
4. Cramer, C.J. *Essentials of Computational Chemistry: Theories and Models*, 2nd ed.; Wiley: New York, NY, USA, 2002.
5. Van Duijneveldt, F.B.; van Duijneveldt-van de Rijdt, J.G.C.M.; van Lenthe, J.H. State of the Art in Counterpoise Theory. *Chem. Rev.* **1994**, *94*, 1873–1885. [CrossRef]
6. Rapaport, D.C. *The Art of Molecular Dynamics Simulation*; Cambridge University Press: Cambridge, UK, 2004.
7. Poltev, V. Molecular Mechanics: Principles, History, and Current Status. In *Handbook of Computational Chemistry*; Leszczynski, J., Ed.; Springer: Dordrecht, The Netherlands, 2015. [CrossRef]
8. Fishman, G.S. *Monte Carlo: Concepts, Algorithms, and Applications*; Springer: New York, NY, USA, 1996.