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Editorial

Recent Progress in Theoretical Studies and Computer Modeling of Non-Covalent Interactions

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It is not at all surprising that the topic of non-covalent interactions, a key pillar of supramolecular chemistry, has seen interest grow enormously within the last decade. There has been significant progress, not only in assessing the synthesis, structure, and properties of functional materials based on non-covalent interactions, but also in the increasing influence of theoretical studies and computer modeling in these regards. In this Editorial, I would like to highlight some of the recently published interesting papers from various MDPI journals that focus on theoretical studies and computer modeling of non-covalent interactions.

In [1], non-covalent interactions responsible for molecular features and self-assembly in naphthazarin C polymorph were investigated on the basis of diverse theoretical approaches: density functional theory (DFT), diffusion quantum Monte Carlo (DQMC), symmetry-adapted perturbation theory (SAPT) and Car–Parrinello Molecular Dynamics (CPMD). In [2], authors raised a question from both experimental and theoretical perspectives: will the non-covalent interactions of some platinum (II)-based drugs (viz. cisplatin, carboplatin and oxaliplatin) with B-vitamins reduce their therapeutic effects in cancer patients? In [3], there was a discussion of the supramolecular diversity of, theoretical investigations into and the antibacterial activity of Cu, Co and Cd complexes based on the tridentate N,N,O-Schiff base ligands. In [4], DFT and wave function theory calculations were carried out in order to to investigate the strength and nature of the intermolecular C-X···N (X = H, Cl, Br, I) bond interactions as a function of the number of cyano groups, CN, in the X-bond donor while maintaining the X-bond acceptor as fixed. The relevance of experimental charge density analysis in unraveling non-covalent interactions in molecular crystals was reviewed and analyzed in [5]. A detailed theoretical investigation of the intermolecular vibrational energy transfer process and the non-covalent intermolecular interactions between explosive compounds were reported in [6]. The chalcogen···chalcogen bonding in molybdenum disulfide, molybdenum diselenide and molybdenum ditelluride dimers as prototypes for a basic understanding of the local interfacial chemical bonding environment in 2D layered transition metal dichalcogenides was discussed in [7]. A theoretical investigation of carbon dioxide adsorption on Li^+-decorated nanoflakes was presented in [8]. The host–guest interactions of cucurbit[7]uril as host and amphetamine, methamphetamine and their enantiomeric forms (S-form and R-form) as guests were computationally investigated in [9] using DFT calculations with the recent D4 atomic charge-dependent dispersion corrections. A theoretical study on the NMR properties of the cyanide anion as a quasi-symmetric two-faced hydrogen bonding acceptor was reported in [10]. Deciphering the hydrogen bonding preference on nucleoside molecular recognition through model copper (II) compounds was presented in [11]. The theoretical study of inter- and intramolecular bifurcated chalcogen bonding in thiadiazole and thiazole-derived diaminocarbene binuclear palladium (II) coordination compounds was discussed in [12]. The paths for the construction of new crystal forms of biologically active compounds via non-covalent interactions (viz. adducts of Nevirapine and Anastrozole with halogen

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bond donors) and a theoretical investigation of the nature and energies of the weak intermolecular contacts responsible for supramolecular self-assembly in the solid state was reported in [13,14]. Theoretical insights into about phosphine oxides as spectroscopic halogen bond descriptors, including IR and NMR correlations with interatomic distances and complexation energy, were analyzed in [15]. Halogen bonding in isostructural cobalt (II) complexes with 2-halopyridines was discussed in [16]. Symmetrical non-covalent interactions between Br···Br, observed in the crystal structure of exotic primary peroxide, were reported in [17]. In [18], a theoretical study demonstrated that non-covalent halogen···halogen interactions play crucial roles in the self-assembly of highly polarizable dichlorodiazadienes, and halogen bonding can dictate a packing preference in the solid state for this class of dichloro-substituted heterodienes, which may represent be convenient tools for a fine tuning of the properties of this novel class of dyes. The phenomenon of bonding interactions in the 1,2-diboraoxazole cycles was theoretically studied via topological analysis of the electron density distribution (Quantum Theory of Atoms in Molecules analysis) in [19]. A theoretical study of *closo*-borate anions $[B_nH_n]^{2-}$ (n = 5–12), including bonding, atomic charges, and reactivity analyses, was presented in [20]. A theoretical insight into the symmetry of salen analogues featuring O-H-N hydrogen bonds was presented in [21]. The Cambridge structural database survey and theoretical considerations of matere bonds in technetium compounds was published in [22]. The effect of metal coordination of selenoxides, themselves being excellent chalcogen bond donors, was analyzed in [23]. A cost-effective scheme for the highly accurate description of intermolecular binding in large complexes was presented in [24]. Chalcogen bonds, stabilizing ligand conformation in the binding pocket of carbonic anhydrase IX receptor mimic, was discussed in [25]. Features of hydrogen bonds and stacking interactions in organotin (IV) complexes of 2-[4-hydroxy-3-((2-hydroxyethylimino)methyl)phenylazo]benzoic acidas, which could be promising antibacterial materials, were discussed in [26]. A comprehensive empirical model of substitution–influence on hydrogen bonding in aromatic Schiff bases was postulated in [27]. A halogen-bonded 2D network, based on a diiminedibromido gold (III) complex and tribromide building blocks was analyzed in as an example of self-assembly of supramolecular architectures driven by σ-hole interactions [28]. In [29], DFT computations revealed that the mechanisms of the asymmetric catalytic reactions of diisopropylzinc with pyrimidylaldehyde were catalyzed by 1- and 2-aza [6]helicenes, making them effective inductors of the autocatalytic chiral amplification Soai reaction, and that generation of chirality takes place through the formation of adducts of aldehyde and of helicenes stabilized via non-covalent dispersion interactions which strictly define the orientation of the aldehyde molecule in the corresponding transition state. A quantum chemical deep dive into the π–π interactions of 3-methylindole and its halogenated derivatives was presented in [30] with the aim of improving ligand design and tryptophan stacking. A computational investigation through the new composite method, r^2SCAN-3c, of the key factors influencing the host–guest interactions was reported in [31]. Insights from DFT, docking, and molecular dynamics simulation studies of halogen-based 17β-HSD1 inhibitors were presented in [32]. A theoretical investigation via DFT and molecular docking of synthesized oxidovanadium (IV)-based imidazole drug complexes, as promising anticancer agents, was presented in [33]. A comprehensive DFT investigation of the adsorption of polycyclic aromatic hydrocarbons onto graphene was published in [34]. Experimental and theoretical deep insights into the structure–property relationship of thermo-induced fluorochromism in zinc complexes were presented in [35]. A computational study of the influence of ionic liquids adsorption on the electronic and optical properties of phosphorene and arsenene with different phases was reported in [36]. The non-covalent functionalization of graphene oxide-supported 2-picolyamine-based zinc (II) complexes, as novel electrocatalysts for hydrogen production, was discussed in [37]. Structural and energetic aspects of entacapone–theophylline–water cocrystal were discussed in [38]. The adsorption of small molecules onto the copper paddle–wheel surface and influence of the multi-reference ground state on these processes were theoretically analyzed in [39]. Finally, various anion-responsive fluorescent

supramolecular gels were theoretically studied in [40]. A comprehensive DFT study of the molecular and electronic structure of metal-free tetrabenzoporphyrin and its metal complexes with Zn, Cd, Al, Ga, and In were presented in [41]. A dispersion-corrected DFT investigation of the inclusion complexation of dexamethasone with β-cyclodextrin and a molecular docking study of its potential activity against COVID-19 was reported on in [42]. A non-covalent dimer formation of a quaternary ammonium cation with unusual charge neutralization in electrospray-ionization mass spectrometry was theoretically analyzed in [43]. Supramolecular halogen-containing capsules were theoretically studied in [44]. An actual symmetry of symmetric molecular adducts in the gas phase, solution and in the solid state was theoretically analyzed in [45]. Various weak noncovalent interactions in cocrystals of isoniazid with glycolic and mandelic acids were theoretically studied in [46]. A comparative DFT study providing new insights into H_2S adsorption onto graphene and graphene-like structures was reported in [47]. A theoretical perspective [48] highlighted the prospects for the application of halogen bonding in organocatalysis. The nature and energies of intermolecular interactions in molecular organic crystals upon the relaxation of lattice parameters were theoretically examined in [49]. Finally, various intermolecular non-covalent carbon-bonding interactions with methyl groups were reviewed in [50] based on comprehensive and systematic evaluations of the Cambridge structural database and the Protein Data Bank in conjunction with DFT calculations.

Of course, these are many more studies in the field of studying non-covalent interactions using theoretical methods and computer simulation. To date, there has been an avalanche-like growth in the number of publications in this direction, and great hopes and prospects for the analysis of big data, machine learning and artificial intelligence in this regard.

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