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Partitioning electrostatic molecular properties into the localized contributions

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Approximations for the molecular dipole moment vector as well as for the spatial distributions of the charge density and electrostatic potential in terms of localized contributions associated with individual atoms and covalent bonds are discussed. The application of recently proposed CLPO method [1] yielding the chemically meaningful set of localized orbitals particularly suitable for this application is considered. The role of the atomic lone electron pairs and bonding orbitals charge densities is highlighted in achieving an accurate decomposition of electrostatic molecular properties into the localized contributions. Comparison with simple point-charge methods, traditionally used in force fields for molecular dynamics simulations, is made. Impact of accuracy of the considered decompositions on electrostatic component of intermolecular interaction energy is quantified for the standard test set of non-covalently bounded complexes GMTKN55 [3].
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[1] T. Y. Nikolaienko and L. A. Bulavin, *Int. J. Quantum Chem.* (2019), **119**: e25798.
[2] L.Goerigk, A.Hansen, C.Bauer, S.Ehrlich, A.Najibi and S.Grimme, *Phys.Chem.Chem.Phys.* (2017), **19**:32184.

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