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Tackling halogen bonds with “simple” force field methods: are we there yet?

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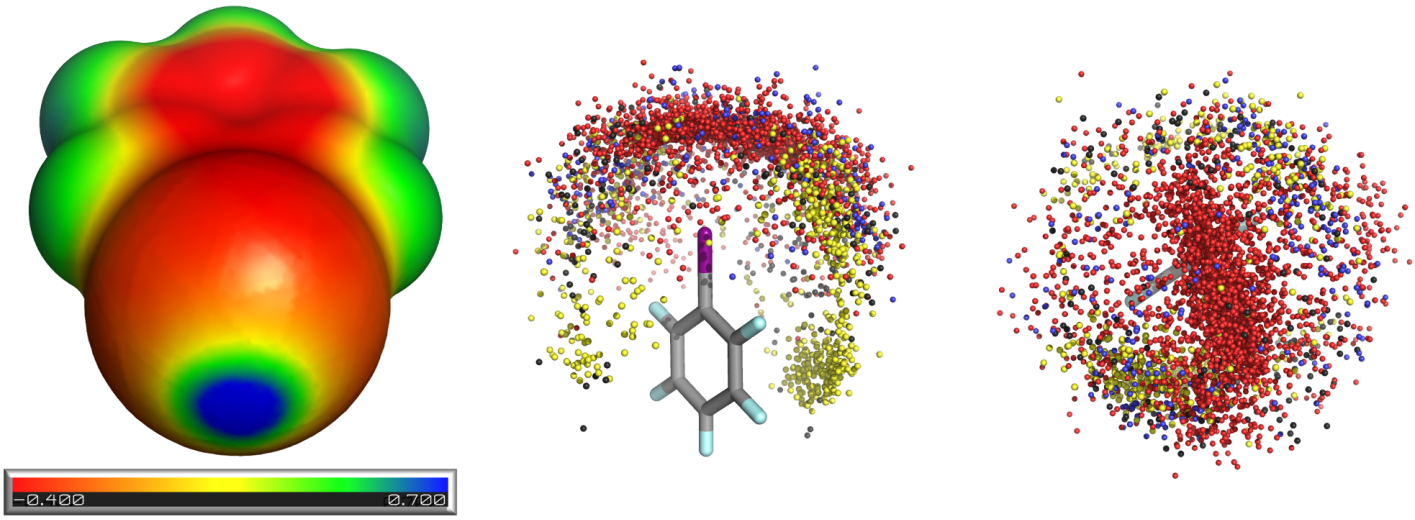

Halogenation of compounds is known to enhance drug properties like membrane permeability and pharmacokinetic stability, playing a significant role in drug discovery. Most strikingly, these compounds also bind to biomolecular targets (proteins, nucleic acids, biomembranes) via an “odd” noncovalent interaction named halogen bond. In this bond, the halogen atom acts as an electrophile and thus, can interact with Lewis bases. Such behavior is due to an anisotropic charge distribution at the halogen, leading to a positive region at the tip of this atom, known as the σ-hole, which can interact with negative sites. Dealing with this charge anisotropy with force-field-based methods, which traditionally use point charges, is not straightforward. In this talk, we will highlight how MD simulations can be used to push the boundaries of halogen bond applications, for instance, to study their influence on membrane recognition and drug permeation, and we will present the latest parameterization efforts to tackle these interactions while also disclosing the current caveats of the methods.