Dynamic Electrostatic Potential

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The computer program PRIOR, which is part of the BayMEM suite [1] is able to calculate a dynamic electron density from a multipole model [2]. Such a density or the result of a maximum entropy method (MEM) calculation can be used to calculate a dynamic electrostatic potential by a modified version of the PRIOR program.

$$\Phi_{static}(\vec{r}) = \phi_{static,rec}(\vec{r}) + \phi_{static,dir}(\vec{r})$$

$$\phi_{static,rec}(\vec{r}) = \frac{1}{\pi V_{UC}} \sum_{H} \frac{F_{static,total}}{|\vec{H}|^2} e^{-2\pi i \vec{H}\cdot\vec{r}} \cdot e^{\frac{-|\vec{H}|^2}{\eta^2}}$$

$$\phi_{static,dir}(\vec{r}) = \sum_{UC} \frac{\rho_{static,total}}{|r - r_{UC}|} erfc(\eta|r - r_{UC}|)$$

The basic idea of the algorithm is based on the Ewald summation [3] were the calculation of the (static) electrostatic potential is divided into a reciprocal and direct space part, applying an arbitrary mixing parameter η which is used to let both parts converge. When dynamic total electron densities are used the reciprocal part of the Ewald summation converges already with η = ∞ so that the direct space part can be omitted. This make this approach quite fast.

We will show applications to organic molecules and boron based solids

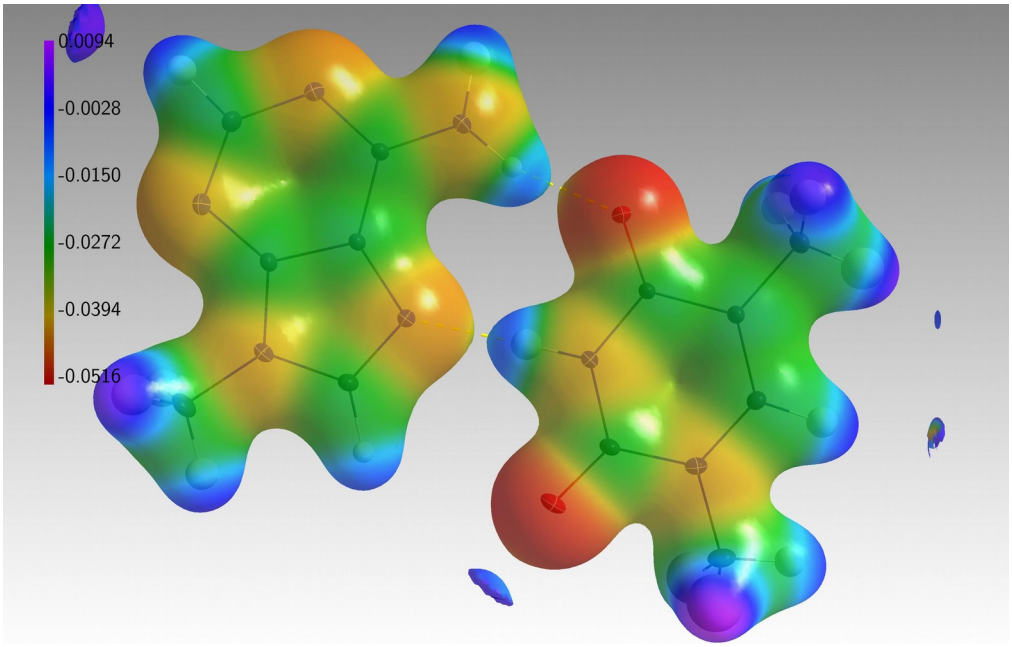

Fig1: Dynamic electrostatic potential of the Hoogsteen base pair *methyl*-Adenine-*methyl*-Thymine maped on the dynamic electron density isosurface at 0.0444 e bohr^{-3}

[1] L. Palatinus, S. van Smaalen and M. Schneider. *Acta Crystallogr.*(2003) **A59** 459-469.

[2] S. Mondal, S. J. Prathapa and S. van Smaalen. *Acta Crystallogr.*(2012) **A68** 568-581.

[3] P. Ewald (1921). “Die Berechnung optischer und elektrostatischer gitterpotentiale.” *Annals*

Phys. **64**, 253-287.