**Parameterization of exchange-repulsion for QM/EFP systems**

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The effective fragment potential (EFP) is a quantum mechanical-based model designed to accurately describe molecular interactions. In EFP the system is fragmented and the interaction energy between fragments is computed as the sum of electrostatics, polarization, dispersion, and exchange-repulsion terms. The computational bottleneck in EFP is the calculation of exchange-repulsion, which is several times more expensive than the other terms. This costly term accounts for repulsion between electrons due to Pauli's exclusion principle, and it is derived from the exact Hartree-Fock energy between non-interacting fragments. In this work we develop a scheme for estimating the exchange-repulsion energy between quantum mechanical (QM) and EFP subsystems by a sum of Gaussian functions with two parameters, $\beta$ and $\alpha$. The first controls the height of the curve, whereas the second determines its width. By finding $\beta$ and $\alpha$ parameters that approximate the exchange-repulsion energy for each unique fragment, significant simplifications in the QM/EFP calculations can be achieved. Such improvement in QM/EFP will facilitate investigating photochemistry in condensed phases.