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Development of the fragment molecular orbital method combined with DFT and DFTB and applications to proteins

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In the fragment molecular orbital method (FMO), a molecular system is divided into fragments, and they are calculated in the electrostatic embedding of the whole system. Most standard quantum-mechanical methods can be used with FMO, including density functional theory (DFT), time-dependent DFT (TDDFT) and density-functional tight-binding (DFTB). The computational cost of FMO is nearly linear, enabling large scale molecular calculations. At the DFT level, that means hundreds or thousands of atoms, and at the DFTB level, a system composed of one million atoms was computed. The methodology of FMO will be briefly introduced and applications will be described, in particular, an application to proteins, which brings up the question of their HOMO-LUMO gap and metallicity of proteins as predicted by DFT and DFTB with some functionals. The role of long range corrections and solvent is very important for describing the electronic state of proteins.

Presenter: Dr FEDOROV, Dmitri (AIST)