Periodic Calculations with NDDO Hamiltonians

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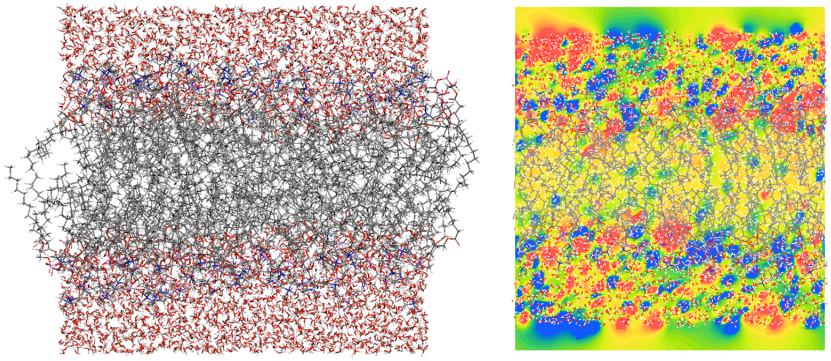
We have implemented periodic boundary conditions (PBC) in the massively parallel semiempirical MO theory code EMPIRE using the cyclic cluster approach. By using sufficiently large unit cells, the calculations are performed entirely in real space. This is easily affordable due to the low computational cost of these methods, and the efficient parallelization of EMPIRE[1].



Specific features of PBCs in EMPIRE include the treatment of very large systems in 1-, 2- or 3D, and the calculation of local properties such as the molecular electrostatic potential and the local electron affinity and ionization potentials. The figure shows the 2D periodic unit cell of a lipid bilayer membrane in water, containing more than 25,000 atoms. On the right, the molecular electrostatic potential of the system is shown on a slice cutting through the unit cell.

[1] M. Hennemann and T. Clark, *J. Mol. Model.* **2014**, *20*, 2331 (11 pages).