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ELECTRODE: An electrochemistry package for atomistic simulations

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The ELECTRODE package is a module in the official release of the molecular dynamics code LAMMPS and implements the constant potential method and related methods. Utilizing the massively parallel architecture of LAMMPS with neighbor lists and fast Fourier transforms, the package efficiently calculates interactions between atoms and minimizes their energy as a function of atom charges.

Standard Ewald summation and the particle-particle particle-mesh algorithm have been implemented for interaction calculations. For the energy minimization, a matrix inversion and the conjugate gradient method can be used.

Numerous research groups have used the ELECTRODE package for atomistic models of supercapacitors, batteries, the electrolyte Seebeck effect and electron transfers at functionalized interfaces. Further, the recently added charge equilibration enables modeling of non-metallic materials.

I want to give a Lightning Talk

yes

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