Submitted: 27 April 2020
Accepted: 06 July 2020
Published Online: 28 July 2020

Simulations of electrolyte between charged metal surfaces

J. Chem. Phys. **153**, 044121 (2020); https://doi.org/10.1063/5.0012073

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We present a new method for simulating ungrounded charged metal slabs inside an electrolyte solution. The ions are free to move between the interior and exterior regions of the slab–electrolyte system. This leads to polarization of both sides of each slab, with a distinct surface charge induced on each surface. Our simulation method is based on the exact solution of the Poisson equation using periodic Green functions. To efficiently perform the calculations, we decouple the electrostatic energy due to surface polarization from that of purely Coulomb interaction between the ions. This allows us to combine a fast 3D Ewald summation technique with an equally fast calculation of polarization. As a demonstration of the method, we calculate ionic density profiles inside an electrolyte solution and explore charge neutrality violation in between charged metal slabs.

ACKNOWLEDGMENTS

This work was partially supported by the CNPq, FAPERGS, and INCT-FCx and by the US-AFOSR under Grant No. FA9550-16-1-0280. M.G. thanks FAPESP under Grant No. 2019/06088-3.

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