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How large are solvent shells for local electronic properties and vibrational spectra in ionic liquids?

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Ionic Liquids (ILs) are known to be promising materials with regard to various different fields, including electrochemistry[1,2] and catalysis, as they ubiquitously share the promising feature of ion conductivity.[3] All the while it is key to understand the underlying molecular behavior and inherent structuring inside these liquids, to efficiently optimize their usage for future applications. The presented analysis regarding locality effects[4,5,6] in ILs is realized using theoretical methods[7,8] and multiple ILs are considered.

By modeling ILs using classical molecular dynamics (MD), the average first and second solvation shell with respect to both anion and cation are characterized as a first step. These results allow to define selection rules regarding the minimal required system size (amount of ion pairs) needed to describe all significant locality effects present in a particular IL. These rules are subsequently tested with respect to their applicability by calculating electrostatic structure properties (charges and dipole moments) and producing vibrational spectra using *ab initio* MD simulations. The quality of the obtained spectra for IL systems of different size will be compared. The findings are then referred back to the idea of locality present in the ILs. The newly derived set of rules is presented as a guideline to obtain spectroscopic quantities in a computationally efficient manner using a combination of classical MD and *ab initio* MD.

References:
[1] M. Salanne, Ionic Liquids for Supercapacitor Applications, Topics in Current Chemistry 2017, 375, 1-25
[2] A. Balducci, Ionic liquids in Lithium-Ion Batteries, Topics in Current Chemistry 2017, 375, 20
[3] B. Clare, A. Sirwadana, D. R. Macfarlane Synthesis, purification and characterization of ionic liquids, Topics in Current Chemistry 2010, 290, 1-40
[4] K. Wendler, S. Zahn, F. Dommert, R. Berger, C. Holm, B. Kirchner, L. Delle Site, Journal of chemical theory and computation 2011, 10, 3040-3044
[5] B. Lambeth Jr, C. Junghans, K. Kremer, C. Clementi, L. Delle Site, The Journal of chem., phys,. 2010, 22, 221101
[6] C Krekeler, F Dommert, J Schmidt, Y. Zhao, C. Holm, R. Berger, L. Delle Site 2010, 12(8), 1817-1821
[7] S. Plimpton, Fast Parallel Algorithms for Short-Range Molecular Dynamics, J. Comput. Chem. 1995,
4, 1-19
[8] J. Hutter, M. Iannuzzi, F. Schiffmann, J. VandeVondele, CP2K: atomistic simulations of condensed matter systems, Comp. Mol. Sci. 2014, 4, 15-25