Spectroscopy of ionic liquids: insights from computer simulations

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In this contribution we present a brief review of the possibilities that computational methods offer to study a wide variety of spectroscopy related magnitudes (Raman/IR spectra, EELS, refractive index…) We particularize for some of the studies carried out in our group on the field of ionic liquids (ILs), with special interest in the understanding of the effects of including metal ions in solvents, both in bulk and near interfaces, to better reproduce and understand the behavior of electrochemistry devices. In a first work we test the accuracy of the parametrization of a force field comparing computational results with experimental Raman spectroscopy data for a bulk system consisting of a mixture of ethylammonium nitrate (EAN) and aluminum nitrate [1]. Then, we show the effects on the spectra and optical properties of some "2D" sheets (graphene, borophene) with the addition of, first, just an IL ([BMIM][BF_4]) [2], and then, the same IL plus a metal (potassium) [3]. Finally, we will show the results of a similar study we are currently working on, that consists of replacing the potassium atom with other metals of different valences and radiuses (Li, Na, Ca, Al).

References:

[1] Gómez-González, V., Docampo-Álvarez, B., Montes-Campos, H., Otero, J. C., Lago, E.L., Cabeza, O., Gallego, Luis J. and Varela, L. M. *Phys. Chem. Chem. Phys.* **20(28)** (2018), 19071-19081.

[2] Zhour, K., Otero-Mato, J. M., Hassan, F. E. H., Fahs, H., Vaezzadeh, M., López-Lago, E., Gallego, L. J., and Varela, L. M. *J. Mol. Liq.* **316** (2020), 113803-113814.

[3] Zhour, K., Otero-Mato, J. M., Hassan, F. E. H., Fahs, H., Vaezzadeh, M., López-Lago, E., Gallllego, L. J., and Varela, L. M. *J. Mol. Liq.* **321** (2021), 114759-114771.