Ab-initio contact area between ions

M. Di Gennaro[1], K. Gkagkas[2] and A. Vernes[3]

[1] Nanomat and Q-Mat, Université de Liege, Belgium; [2]Material Engineering Division, Toyota Motor Europe NV/SA, Zaventem, Belgium; [3]AC2T research GmbH, Wiener Neustadt, Austria and Institute of Applied Physics, TU Wien, Vienna, Austria

E-mail: andras.vernes@ac2t.at

With the introduction of the density-functional theory (DFT) more than fifty-five years ago, a revolutionary epoch started in both quantum mechanics and computational chemistry, since the main advantage of DFT is its universality, namely that it is equally well suitable to describe the electronic structure of atoms, molecules as well as liquids or solids [1]. Additionally, by computing the gradient of the DFT-calculated electronic density, it is also possible to fully characterize any nanoscopic system of interest from a topological point of view within the so-called Quantum Theory of Atoms in Molecules (QTAIM) [2]. Taking advantage on QTAIM, it was demonstrated that the separation area between contacting atoms and its dependence on distance can be straightforwardly estimated [3]. In this contribution, the load dependence of the *ab-initio* contact area between the constitutive ions of two EMIM-based ionic liquids is determined and shown its formal similarity with those of the adhesive contact models well known at the macroscopic length scale, see Fig. 1. This numerical finding is expected to aim for correlating tribochemistry with contact mechanics.

References

[1] R. M. Martin, *Electronic Structure – Basic Theory and Practical Methods* (Cambridge University Press, 2020).

[2] R. F. W. Bader, J. Mol. Struct: THEOCHEM 943, (2010) 2.

[3] M. Wolloch, G. Feldbauer, P. Mohn, J. Redinger, and A. Vernes, Phys. Rev. B 91 (2015) 195436.

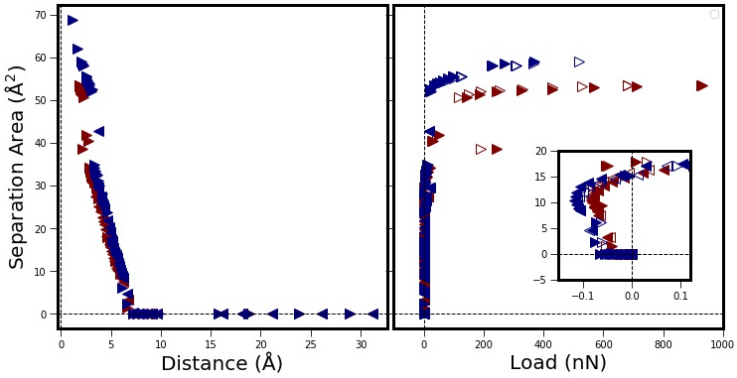

Fig. 1 *Ab-initio* contact area between the ions for EMIM-BF4 (red) and EMIM-PF6 (blue).