Área: FIS

A Molecular Dynamics Simulation Study on the Stability of Gold Nanoparticles in Ionic Liquids

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Highlights

Ionic liquids are organized in layers of ions when gold nanoparticles are close to each other. When long alkyl chains are present in the side chain of cation, an apolar layer between two gold nanoparticles arises, which requires up to 90 kJ mol^{-1} to be broken and is likely responsible for the stability of gold nanoparticles in ionic liquids.

Resumo/Abstract

Gold nanoparticles have high superficial area and possess interesting magnetic and electronic properties. Ionic liquids (IL) are room temperature molten salt and have been widely studied electrolytes for supercapacitors/batteries, as solvent for catalysis, synthesis and stabilization of metal nanoparticles, for instance, gold nanoparticles. Ionic liquids are expected to act as electronic and steric stabilizers.[1,2] However, a detailed description of how the stabilization takes place is still scarce. Therefore, we performed molecular dynamics simulations of two gold nanoparticles (NP) immersed in 4 IL ([EMIM][BF_4], [EMIM][NTf_2], [OMIM][BF_4] e [OMIM][NTf_2]) with the GROMACS program. The liquids were simulated with CL&P force field [3], while the NP were simulated with a previous model proposed by Heinz [4]. The potential of mean force calculated to bring one NP to another is characterized by oscillations of small energy barriers that are related to the squeeze out of layers of ions in between the NPs when the ILs have short chain (EMIM-based IL). When long alkyl chains are present in the side chain of cation, an apolar layer between two gold nanoparticles arises, which requires up to 90 kJ mol^{-1} to be broken and is likely responsible for the stability of gold nanoparticles in ionic liquids.

References

1) Z. He e P. Alexandridis. Physical Chemistry Chemical Physics, 17 (28), 18238 – 1826, 2015.

2) K. J. Mohammed, S. K. Hadrawi e E. Kianfar. BioNanoScience 13 (2) 760–783, 2023.

3) J. N. Canongia Lopes and A. Pádua, Theoretical Chemical Accounts 131, 2012.

4) Heinz, H.; Vaia, R. A.; Farmer, B. L.; Naik, R. R. J. Phys. Chem. C 112, 17281–17290, 2008.

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