

Na⁺/Cu⁺ rivalry in neutral organic solvents and on an inert surface
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Copper is utilized not only as the perfect current collector but also as a supporting frame for graphene (or rGO) sheets used as anodes in sodium-ion batteries. However, the solvent's polarity influences the efficiency of the cell and since XPS studies prove the emergence of copper on the electrode surface, its origin in the system and the dependence on the solvent used call for elucidation. The present study aims to provide a comparative theoretical (DFT) analysis of the interactions of the monovalent cations Na⁺ and Cu⁺ in neutral organic solvents with different polarity – diglyme ($\epsilon = 7.3$) and propylene carbonate ($\epsilon = 64.9$). The main objective is to evaluate the energetics of solvation and adsorption to the end of rationalizing the experimental findings.