Exploring the Interactions Between Graphene Oxide and Deep Eutectic Solvents: A Combined Experimental – Theoretical Approach

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Deep eutectic solvents (DESs) are an emerging class of eutectic mixtures known for their low cost, low toxicity, and highly tunable physicochemical properties, such as adjustable polarity, thermal stability, and strong solubilizing capabilities. These characteristics make DESs attractive in fields ranging from green chemistry to materials processing. Particular attention is being directed toward their interaction with two-dimensional (2D) materials like graphene oxide (GO), which features high surface area, tunable oxygen-containing functional groups, and excellent dispersibility—attributes central to applications in catalysis, energy storage, and bioelectrochemical devices.

However, the fundamental mechanisms governing DES-GO interactions remain underexplored. In this study, we investigate the structural and interfacial behavior of two representative DESs - ethaline (choline chloride:ethylene glycol) and reline (choline chloride:urea) - in contact with GO, through a combination of thermal and vibrational characterization techniques. Differential scanning calorimetry (DSC) was used to assess phase behavior and stability, while mid- and far-infrared spectroscopy enabled a detailed analysis of intra- and intermolecular interactions, including hydrogen bonding and structural rearrangements induced by DES adsorption on GO.

To support the experimental findings, molecular dynamics (MD) simulations were performed using a GO model derived from X-ray photoelectron spectroscopy (XPS) data on the same synthesized material. Radial distribution functions (RDFs) were calculated to probe the local arrangement and affinity of DES components at the GO interface. The integration of experimental and computational results offers new insights into the molecular-scale mechanisms driving DES-GO interactions, supporting the rational design of DES-based nanocomposites for advanced technologies.

Francesco Trequattrini earned the degree of "Doctor in Physics" from the University of Perugia. Since 1993 he has been a permanent researcher at the University of Rome "La Sapienza", where he teaches at the Faculty of Engineering and conducts his research at the Department of Physics. He is co-author of 140 peer-reviewed publications in international journals and contributed a chapter to the book *Tunneling Systems in Amorphous and Crystalline Solids* (Springer). **Google Scholar**: h-index 25, i10-index 64, Citations: 2117.