Interstellar Life Quest: Gold-Water Simulation

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Interstellar icy layers on dust grains are critical venues for astrochemical reactions, influencing the fates of celestial entities and even life itself. These layers, mostly composed of water, catalyze some vital astrochemical processes. However, the effect of temperature on these processes is usually overlooked, despite the importance. Gold, recognized for its thermal conductivity, serves as a model substrate, but its high cost and difficulty of regulating low temperatures limit investigation. A previous study depicted that gold facets also cause differences in icy layer's structural properties. Molecular dynamics, molecular mechanics, and density functional theory calculations under periodic boundary conditions were used to investigate icy layer formations on several gold facets ((111), (110), (100), and (511)). Lennard-Jones and Morse potentials were chosen for the classical approach as implemented in gulp and dlpoly ,and GGA-PBE/PWscf with PAW pseudopotential was used for the DFT calculations implemented in quantum espresso. Our computational work were checked against a reported literature which the interaction energies from both methods were consistently found to converge to the ice cohesive energy. We revealed a set of parameters that govern the formation of these icy layers, which are crucial for the catalytic activity of the fundamental astrochemical events. Interestingly, our work suggests that icy layer can be formed properly under the optimal values of water layer's thickness (15-25 Å, ~10 layers) and temperature (~40 K). Leveraging these results, we are working on mimicking ribose formation, a key process in the study of the origin of life, on the icy layer, bridging a research gap where high barrier energy in gas-phase reaction makes it nearly impossible.