

Dynamics of encapsulated water inside Mo132 cavities

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Abstract

The behavior of liquids is distorted under confinement with respect to their bulk counterpart. We have studied the structure and dynamics of water confined inside almost rigid polyoxomolybdate molecular clusters of the type $[\{(Mo)Mo_5O_{21}\}_{12}\{Mo_2-(ligand)_{30}\}]^{n-}$ by means of classical molecular dynamics simulations under ambient conditions [1]. We observe that water organizes in concentric layered structures of the buckyball family, which agree with X-ray data for these systems at low temperature. Several structural and dynamical data are provided and compared to experimental and theoretical analyses for reverse micelles of similar size, where qualitative agreement is observed. Our results reveal the importance of the competition between the confinement and the long-range structure induced in this system by the hydrogen bond network.

[1] García Ratés *et al.* J. Phys. Chem. B (2011), **115**, 5980–5992