Modelling Hydroquinone Clathrates with Molecular Simulation and Density Functional Theory

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Organic clathrates have demonstrated many interesting features indicating their potential interest in applications such as CO₂ capture and storage, gas separation, or even hydrogen storage. The number of existing organic clathrate formers and crystalline structures is very large, and the complexity of its practically unexplored phase behavior must be emphasized. Their theoretical description is still very unsatisfactory, so modelling of these types of inclusion compounds is a highly desirable objective. In this case, a combined modelling approach has been attempted, using electronic Density Functional Theory (DFT) and the Quantum Theory of Atoms in Molecules (QTAIM), but also molecular dynamics, to describe hydroquinone clathrates. This combined approach has been recently used to describe molecular features of hydrates [1, 2] as potential energy landscapes, preferential guest orientation, and diffusion barriers, geometrical details, and also phase equilibria boundaries as the three-phase coexistence line, or cavity occupancy rates. CH₄ and CO₂ have been considered as guest molecules in this case, analyzing the differences in the clathrate structure and behavior produced, a subject that has been experimentally pointed out only very recently.

References:

[1] A. Vidal-Vidal, M. Pérez-Rodríguez and M. M. Piñeiro, RSC Advances 6, 1966, 2016

[2] M. Pérez-Rodríguez, A. Vidal-Vidal, J. M. Míguez, F. J. Blas, J.-P. Torré and M. M. Piñeiro, Phys. Chem. Chem. Phys. 19, 3384, 2017