Modeling the properties of biogenic crystals using DFT and electrostatic embedding: the case of guanine

Parfaite Senou[1], Carlo Adamo[1], and Frédéric Labat[1]

[1] *Chimie ParisTech, PSL University, CNRS, Institute of Chemistry for Life and Health Sciences, Chemical Theory and Modelling Group, 11 rue Pierre et Marie Curie, Paris, 75005, FR, France*

parfaite.senou@chimieparistech.psl.eu

ABSTRACT

Biogenic crystals are biologically formed molecular crystals that play a key role in various optical phenomena based on light reflection and scattering, such as animal coloration and vision.[1] Among the reflective materials, guanine crystals have been identified in a wide variety of organisms with different morphologies related to specific optical effects, ranging from camouflage to dramatic color changes in the chameleon for example.[2] To date however, the relationship between the structure and properties of these crystals remains largely unexplored. In this contribution, we present an investigation of three previously-proposed crystalline polymorphs of guanine (α, β and γ) and identify a fourth one (γ'). Their structural, electronic, and vibrational properties have been investigated using periodic DFT, while their optical properties have been studied with TD-DFT combined with electrostatic embedding techniques, to simulate their UV-Vis spectra. While computed data were found to be in very good agreement with available experimental data in all cases, no significant differences between the four polymorphs could be identified for their optical properties, despite significant structural differences. This outlines the need to consider a broader polymorphism of such crystals, to decipher the link between their structures and their peculiar properties.

References

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