MARVEL

THEOS
THEORY AND SIMULATION OF MATERIALS

ÉCOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE

Molecular crystal structure prediction with evolutionary algorithm

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Abstract: Accurate ab initio crystal structure prediction of even small organic compounds has been extremely challenging, not only due to polymorphism and molecular flexibility but also due to difficulties in addressing the inter-molecular van der Waals interaction from first principles. [1]
Functionals that describe this interaction have been implemented within Quantum Espresso open source simulation package [2] and their success in predicting the right energy ordering of small organic crystals has been recently demonstrated [3].
In this work we combine this development with the latest tools in the field of evolutionary structure prediction for molecular crystals [1] and asses the applicability, strengths and weaknesses of this combination in the challenging test cases of glycine and cholesterol crystals. Our results not only validate previous findings but also answer open questions and predict new features in the phase space of these molecules, demonstrating the promising future of evolutionary algorithms with ab initio methods.

[1] Zhu, et al., Acta Cryst. B68, 215-226 (2012).
[2] Giannozzi, et al., J. Phys.: Condens. Matter, 21, 395502 (2009).
[3] Sabatini, et al., J. Phys.: Condens. Matter 24, 424209 (2012).