Abstract Submitted
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Ab initio NMR Confirmed Evolutionary Structure Prediction for Organic Molecular Crystals CONG-HUY PHAM, International School for Advanced Studies (SISSA), Trieste (Italy), EMINE KUCUKBENLI, Ecole Polytechnique federele de Lausanne (EPFL), Lausanne (Switzerland), STEFANO DE GIRONCOLI, International School for Advanced Studies (SISSA), Trieste (Italy) — Ab initio crystal structure prediction of even small organic compounds is extremely challenging due to polymorphism, molecular flexibility and difficulties in addressing the dispersion interaction from first principles [1]. We recently implemented vdW-aware density functionals and demonstrated their success in energy ordering of aminoacid crystals [2]. In this work we combine this development with the evolutionary structure prediction method [1] to study cholesterol polymorphs. Cholesterol crystals have paramount importance in various diseases, from cancer to atherosclerosis. The structure of some polymorphs (e.g. ChM, ChAl, ChAh) have already been resolved while some others, which display distinct NMR spectra and are involved in disease formation [3], are yet to be determined. Here we thoroughly assess the applicability of evolutionary structure prediction to address such real world problems. We validate the newly predicted structures with ab initio NMR chemical shift data using secondary referencing for an improved comparison with experiments [4]. [1]Zhu et al. Acta Cryst B68, 215 (2012) [2]Quantum ESPRESSO, Sabatini et al. J Phys Cond Matt 24, 424209 (2012) [3]Jayalakshmi et al. SS Nucl Magn Res 36, 60 (2009) [4]Kucukbenli et al. JCP A 116, 3765 (2012)

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