Precise characterization of the low temperature structures of vanadium oxides

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Vanadium pentaoxide is a van der Waals material that has been used in a variety of applications such as sensors, photocatalysts, electrochromic devices and, more extensively, as cathodes for lithium-ion batteries because of their low cost and abundance [1]. Due to its layered structure, the number of layers can be controlled easily either by exfoliation or by their growth process. Furthermore, it can be easily doped by the introduction of intercalated alkaline and alkaline earth atoms such as lithium, calcium or sodium.

Particularly, the one doped with sodium (NaV2O5), generated a lot of excitement in the early 90s due to its very rich landscape of properties at high and low temperatures. Although its high temperature structure has been known for a long time, the low temperature structure has generated a huge debate that continues nowadays [2-5].

In this work, we want to characterize the low temperature structure of this family of compounds using density functional theory and the stochastic self-consistent harmonic approximation [6].

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