

Dear Editor,

please find in the following point by point description of our amendments.

Point 1 – from line 296 to line 305:

The different performance of the B3LYP and B3LYP-D* approaches in calculating the diagonal and off-diagonal components of the stiffness tensor depends on the underlying physics of the elastic response. The diagonal elastic constants are dominated by the response of the strongly bonded T–O–T layers. When dispersion is neglected (B3LYP), long-range interactions are underestimated, leading to an overexpanded interlayer region. In Gaussian basis-set calculations, this effect partly compensates the overestimation of forces caused by Pulay stress (as discussed below), producing a seemingly better agreement for the diagonal terms. In contrast, the off-diagonal terms describe shear-normal coupling and interlayer-intralayer stress transfer, which are very sensitive to the correct description of weak interactions. Without dispersion (B3LYP), the layers are very decoupled, and the coupling terms $C_{\alpha\beta}$ ($\alpha \neq \beta$) are underestimated or show incorrect relative magnitudes. However, including dispersion (B3LYP-D*) it restores realistic interlayer distances and mechanical coupling, improving the prediction of the off-diagonal elastic constants.

Point 2 – line 409:

The following references along the text are added: (Pavese et al., 2003; Chheda et al., 2014).

I hope the manuscript is now suitable for publication.

My best wishes,

Giovanni Valdrè

Prof. Giovanni Valdrè

Department of Biological, Geological and Environmental Sciences

Piazza di Porta San Donato 1 – 40126, Bologna, Italy

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