Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Benchmarking dispersion-corrected DFT methods for the evaluation of materials with anisotropic properties: structural, electronic, dielectric, optical and vibrational analysis of calcite ($CaCO_3$, space group $R\bar{3}c$)

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Supplementary Materials

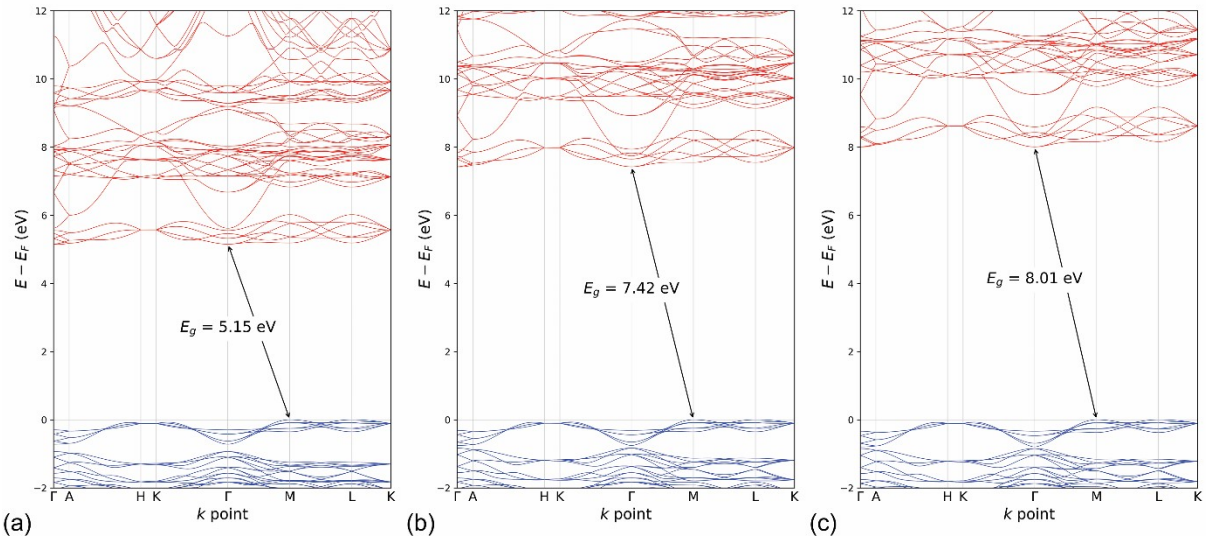

Fig. S1 Band structure of calcite $CaCO_3$, as calculated at DFT level with (a) PBE, (b) B3LYP and (c) PBE0 Hamiltonians. In each panel, the direct band gap is highlighted by a double-headed arrow. Shape and form of bands are not discussed in the present work.