

**Revisiting the importance of dye binding mode in dye-sensitized
solar cells: a periodic viewpoint**

– **SUPPLEMENTARY MATERIAL** –

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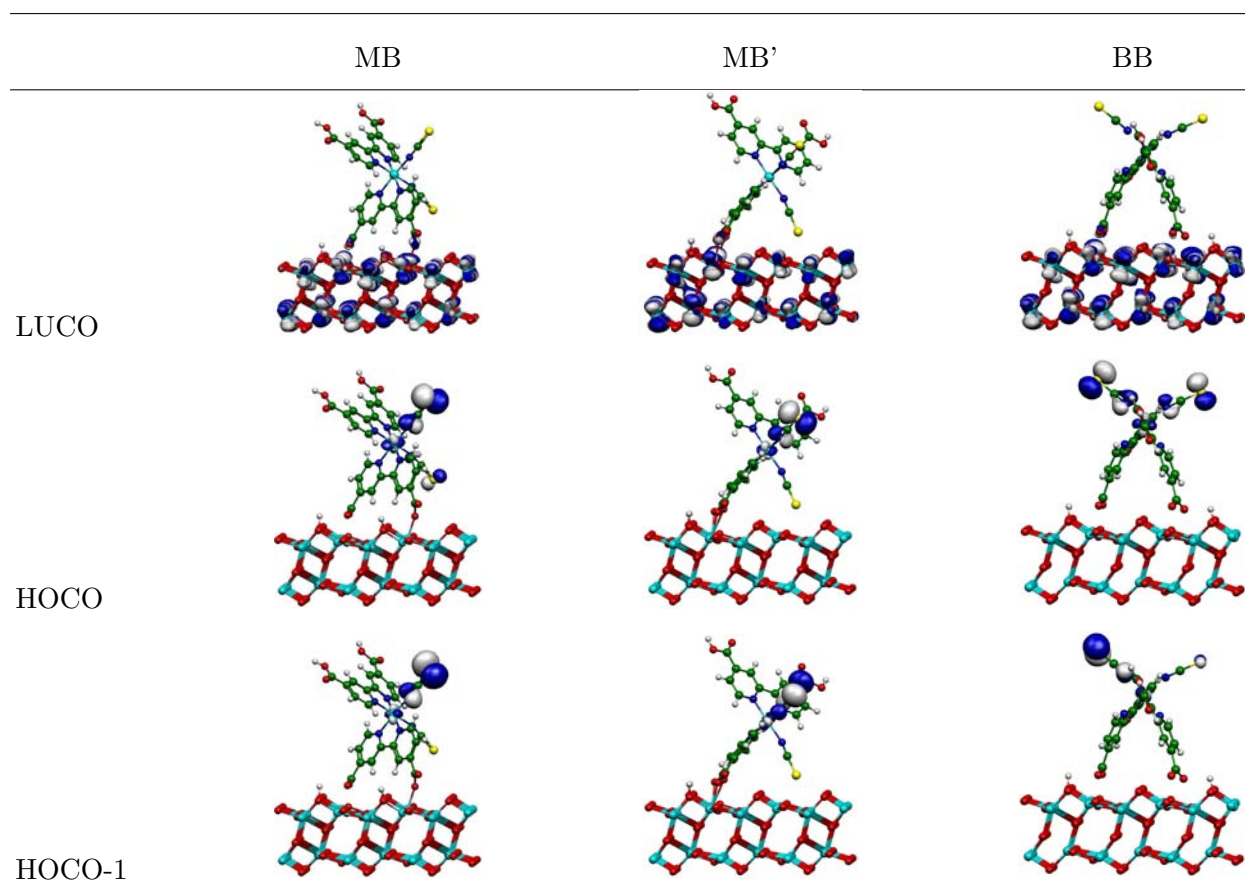


TABLE S1: Computed Γ -point frontier crystalline orbitals for all investigated adsorption modes of N3 on TiO₂ anatase (101). Isovalues: $|0.040|$ and $|0.007|$ for HOCOs and LOCO, respectively.

Fig. S1: Labat *et al.*

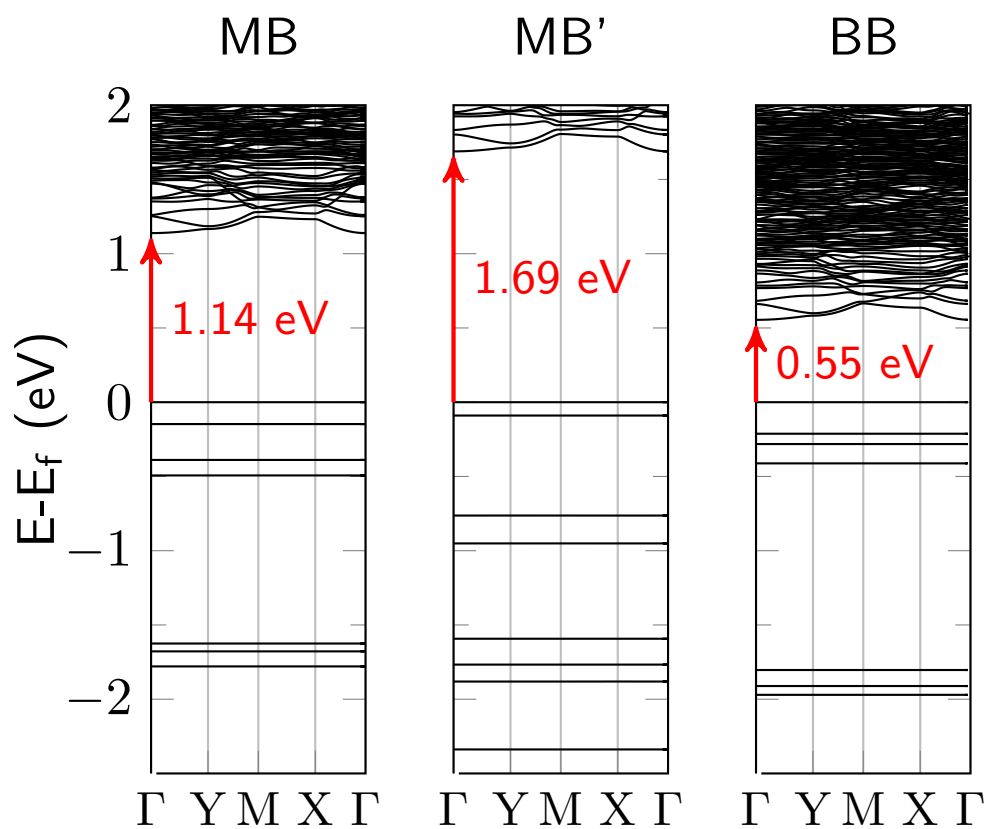


FIG. S1: Computed band structures of the three considered adsorption modes of N3/TiO₂.

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