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Title: Atomic level understanding of site-specific interactions in Polyaniline/TiO<sub>2</sub> composite

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**Highlights:**

- Ti-facing PANi conformation is energetically more preferred than O-facing PANi.
- Bader's charge analysis confirms that there is charge transfer from PANi to TiO<sub>2</sub>.
- There is dependency of the conduction band minimum on the site of TiO<sub>2</sub> interaction.
- pCOHP analysis shows the nature of bonding is different at different interaction sites.

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