Abstract Submitted
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Electronic structure of V-doped TiO2 YUSHAN WANG, University of Delaware — First-principles calculations using the full-potential linearized augmented plane-wave method have been performed to investigate the electronic structure of V-doped TiO2 in the anatase modification. In calculations with local density approximation (LDA) plus U (Hubbard coefficient) approach, V 3d states were found to be completely spin- polarized with net magnetic moment generated.

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