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Electronic Structure of N-doped TiO JAMES LEWIS, BARRY HAYCOCK, GARY LANDER, West Virginia University, Morgantown, WV 26501, United States, BINAY PRASAI, DAVID DRABOLD, Ohio University, Athens, OH 45701, United States — Via *ab-initio*density functional theory calculations, we present evidence of the most energetically stable atomic configuration for nitrogen-doped amorphous TiOand analysis of the electronic structure. This material receives much attention in the literature due to it's proposed photocatalytic applications, however synthesis of the crystalline form is an unfavorable process. Nitrogen doping has previously been shown to enable absorption in the visible in crystalline TiO2. As compared to crystalline TiO2, thin films of a- TiOdo not need thermal treatment and have other production advantages such as less dependence on substrate materials. With control of the electronic structure of the amorphous phase via doping the electronic characteristics can be taken advantage of without the costly production of crystalline TiO. N-doping of the amorphous phase introduces tail states to the valance band.

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