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Origin of the Anatase to Rutile Conversion of Metal-Doped TiO2[1]

SA LI, Virginia Commonwealth University, PURU JENA, VIRGINIA COMMONWEALTH UNIVERSITY TEAM — Extensive calculations using density functional theory enable us to explain the origin of the surprising room-temperature conversion of anatase to rutile phase of TiO2 when doped with Co and Ni, but not with Cu. Contrary to earlier suggestion, neither high spin nor strain of the transition metals is found to be responsible for this phase conversion. The driving mechanism, instead, is attributed to the increased interaction between Co and Ni atoms forming a linear chain in the rutile phase. We predict that Cr and Mn which have even larger spins than Co and Ni cannot induce this phase conversion.

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