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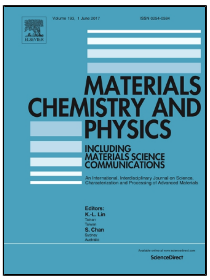

Tuning Electronic Structure and Optical Properties of $SrTiO_3$ by Site-specific doping by Nb with N/B from hybrid functional calculations

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A systematical study has been employed on $SrTiO_3$ with the donor- acceptor codoping. > The donor-acceptor pair codoping yields the absorption edge extend to visible light. > The formation energy implies that the codoped systems are favorable under the O-rich condition. > The Nb@Ti/N@O system is desirable for the spontaneous water splitting under visible light. > The Nb@Sr/B@O system can split water into hydrogen in presence of sacrificial agent.