Rh-doped BaTiO3: Optical and Catalytic Properties

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BaTiO₃ is a ferroelectric oxide widely studied for its applications in non-linear optics, dielectric ceramics, and piezoelectric materials. Recent research has focused on the optical properties of both bare and Rh-doped BaTiO₃ in its tetragonal phase, employing density functional theory. In our investigation of a static lattice, we utilized the generalized gradient approximation combined with on-site Hubbard correlations and a hybrid functional. It is found that accounting for atomic motion significantly reduces the calculated threshold energy for optical absorption. This reduction occurs for two primary reasons. First, thermal motion alters the atomic configuration, causing electronic transitions that are normally "dark" in a static lattice to become "bright." Second, the fluctuations in atomic motion lead to variations in the energy of electronic transitions, further decreasing the optical absorption threshold. Rh-doping enhances BaTiO₃'s light absorption capability while also reducing the overpotential needed for water oxidation. Research indicates that a TiO₂-terminated BaTiO₃ (001) surface shows great promise as a catalyst. Rh doping expands the range of absorbed light to cover the entire visible spectrum. Additionally, the presence of water significantly influences the ability of Rh-doped BaTiO₃ to absorb solar radiation. When Ti is replaced by Rh, the doping ion can acquire some electron density from neighboring oxygen ions. As a result, during the water oxidation reaction, Rh ions may exist in an intermediate oxidation state between 3+ and 4+. This change affects the adsorption energy of reaction intermediates on the catalyst's surface, ultimately lowering the overpotential.

References

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