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Paper title: Lattice dielectric properties of rutile TiO_2: First-principles anharmonic self-consistent phonon study
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Dear Editors of Physical Review B

We are submitting a paper entitled "Lattice dielectric properties of rutile TiO_2: First-principles anharmonic self-consistent phonon study" for consideration of publication as Regular Article in Physical Review B.

Titanium dioxide (TiO_2) in the rutile structure is an incipient ferroelectric material, which shows remarkably large dielectric constants of 110 and 250 along the x and z axes, respectively. The consequent high refractive index has important applications, such as pigments and capacitors. When one studies its dielectric properties theoretically, however, its strong lattice anharmonicity has to be incorporated for accurate analysis. The self-consistent phonon theory makes it possible to deal with such strong anharmonicity, combined with a recently developed *ab initio* computational framework of phonon anharmonicity.

We use *ab initio* anharmonic lattice dynamics methods to investigate the lattice dielectric properties of rutile TiO_2. We employ the modified self-consistent approach, including third-order anharmonicity as well as fourth-order anharmonicity. We also include the four-phonon scattering process for phonon linewidth. We point out that neither the harmonic approximation nor the perturbation method suffices for lattice optical properties. Furthermore, by incorporating the frequency dependence of phonon linewidth, we found that two-phonon emission process is responsible for experimentally known but unidentified peaks of the dielectric function.

Our calculation very well agrees with experimental values and highlights the importance of the self-consistent method and the frequency dependence of phonon linewidth. We therefore believe the present manuscript warrants publication as Regular Article in Physical Review B to appeal to the condensed matter physics community.

Sincerely yours,

On behalf of all the authors,
Tomohito Amano