

# Electron-phonon interactions in oxide materials from first principles: implications for exciton properties and superconductivity

Antonios M. Alvertis

Physics Department and Oden Institute for Computational Engineering & Sciences, The University of Texas at Austin

Polar metal oxides form an ideal testbed for electron-phonon physics. The strong ionic character of these materials produces a stark contrast between the static dielectric constant  $\epsilon_0$ , which includes ionic contributions, and the high-frequency dielectric constant  $\epsilon_\infty$ . This in turn results in significant long-range Fröhlich coupling between charge carriers and longitudinal optical phonons.

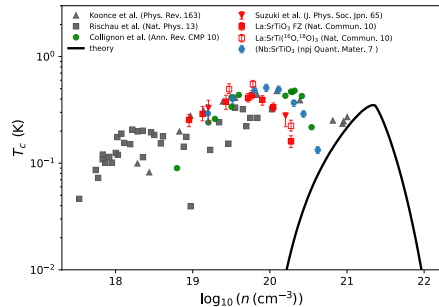


Figure 1: Superconducting dome of SrTiO<sub>3</sub> from experiment and first-principles theory (Ref. [2]).

Apart from mediating the formation of Cooper pairs, as in SrTiO<sub>3</sub>, this interplay of Fröhlich interaction and strong deformation potential coupling that is present in several oxides, can have a strong impact on the excited state properties of these materials. I will present a first-principles theory for including phonon effects in excitonic calculations within the GW-BSE framework [3], and apply it to a range of oxides that include MgO, TiO<sub>2</sub>, BiVO<sub>4</sub>, and SrTiO<sub>3</sub>. I will demonstrate that this results in greatly improved agreement to experiment for a number of quantities, including the exciton binding energy and the optical absorption spectra [3,4].

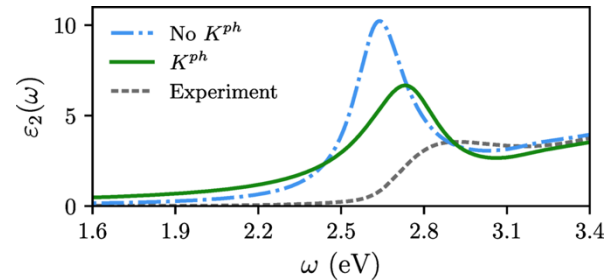


Figure 2: Optical absorption spectrum of BiVO<sub>4</sub> from theory without phonons ( $K^{ph}$ ), including phonons, and experiment. Taken from Ref. [4].

I will close my talk with a discussion of the validity of perturbation theory for electron-phonon interactions in oxide materials, which is almost universally employed in theoretical studies. I will show that low-order perturbation theory can frequently fail catastrophically, and I will present an approach for incorporating non-perturbative electron-phonon interactions from first principles, which results in large corrections to excited state properties in a wide range of properties, compared to low-order perturbative approaches [5].

## References

- [1] Tubman, Coveney, ..., Alvertis, Physical Review B 113, 245144 (2026)
- [2] Coveney, Tubman, ..., Alvertis, arXiv:2501.17230
- [3] Alvertis, Haber, Li, Coveney, Louie, Filip, Neaton, PNAS 121, e2403434121 (2024)
- [4] Gant, Alvertis, Coveney, Haber, Filip, Neaton, Physical Review Research 8, 013105 (2026)
- [5] Lozano Mayo, Alvertis, In Preparation (2027)