Department of Physics

Condensed Matter Physics Clarendon Laboratory, Parks Road, Oxford OX1 3PU



CONDENSED MATTER PHYSICS SPECIAL SEMINAR

Friday 28 November at 14:30
Simpkins Lee Seminar Room, Department of Physics
(https://maps.app.goo.gl/WjG71uLF2D48n85B6)

Importance of lattice screening in condensed matter: from excitons to superconductivity

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The screened Coulomb interaction is a central quantity in condensed matter, which determines critical properties of materials. The formation of bound excitons, Cooper pairs, and exotic states of matter, all depend on the strength of the interaction between electrons and holes, which is screened by the surrounding medium. The vast majority of theoretical approaches consider the screened Coulomb interaction in the presence of a frozen lattice of atoms. However, as suggested by a simple Lorentz oscillator model, atomic motion can greatly modify the properties of the screened Coulomb interaction.

In this talk I will discuss recent theoretical developments that rigorously account for lattice screening in diverse condensed matter systems. First, I will introduce a novel first-principles framework for incorporating lattice screening effects on excitonic properties, which leads to highly temperature-dependent exciton binding energies [1]. This phenomenon is particularly pronounced in low-dimensional heterostructures [2], and explains both the temperature-dependent exciton binding of halide perovskites and ultra-fast exciton dissociation in efficient photocatalysts [3].

I will then show how the effect of phonons on the screened Coulomb interaction can greatly modify the electronic phase diagrams of diverse strongly-correlated materials [4], and explain superconductivity in SrTiO₃ – a long-standing open problem since its discovery in 1964 – through a cooperative mechanism of long-range coupling to multiple longitudinal optical phonons [5].

- [1] Antonios M. Alvertis, Jonah B. Haber, Zhenglu Li, Christopher J.N. Coveney, Steven G. Louie, Marina R. Filip, Jeffrey B. Neaton. "Phonon screening and dissociation of excitons at finite temperatures from first principles". *Proceedings of the National Academy of Sciences* 121, e2403434121 (2024)
- [2] Woncheol Lee, **Antonios M. Alvertis**, Zhenglu Li, Steven Louie, Marina R. Filip, Jeffrey B. Neaton, Emmanouil Kioupakis. "Phonon screening of excitons in atomically thin semiconductors". *Physical Review Letters* 133, 206901 (2024)
- [3] Stephen E. Gant, **Antonios M. Alvertis**, Christopher J.N. Coveney, Jonah B. Haber, Marina R. Filip, Jeffrey B. Neaton. "Ultrafast Spontaneous Exciton Dissociation via Phonon Emission in BiVO₄". arXiv: 2504.00110 (2025)
- [4] Norm M. Tubman, Christopher J.N. Coveney, Chih-En Hsu, Andres Montoya-Castillo, Marina R. Filip, Jeffrey B. Neaton, Zhenglu Li, Vojtech Vlcek, **Antonios M. Alvertis**. "Theory of *ab initio* downfolding with arbitrary range electron-phonon coupling". arXiv: 2502.00103 (2025)
- [5] Christopher J.N. Coveney, Norm M. Tubman, Chih-En Hsu, Andres Montoya-Castillo, Marina R. Filip, Jeffrey B. Neaton, Zhenglu Li, Vojtech Vlcek, **Antonios M. Alvertis**. "Phonon-mediated electron attraction in SrTiO₃ via the generalized Frohlich and deformation potential mechanisms". arXiv: 2501.17230 (2025)

Host: Professor Marina Filip