



Exciton-phonon coupling from first principles

Claudio Attaccalite

CNRS concours 03/01 (2021)

Short CV 1/2



2001: Master in Physics, La Sapienza University (Rome)

2005: PhD in Physics, SISSA, Trieste (Italie) *S. Sorella*

2006-2007: PostDoc, IEMN, Lille, *L. Wirtz*

2008-2009: PostDoc, Universidad del Pais Vasco, *A. Rubio*

2009-2014: CNRS Researcher (CR2), Institute Néel, France

2014-2018: CNRS Researcher (CR1), CINaM, France

2018-2019: Visiting Researcher, Tor-Vergata Univ. (Rome)

Short CV 2/2



PostDoc/Phd supervision:



2 postdocs,
3 Phd,
3 master, 2 internship

ANR, Aix-Marseille Univ.,
Region Rhone-Alpes,
Tor Vergata Univ., HPC-Europe

Short CV 2/2



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Scientific Production:



53 papers, 1 patent
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H-index 28

15 invited talk, 13 talk
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Statistical Mechanics (18/19)
Density Func. Theory (2017)
7 International Schools(2008-)



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1 School
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Editor Fellow for SciPost.org

Comité de direction:

GDR-REST, ETSF, COST-
Action CA17126



Comité scientif. GDR-HOWDI
Correspondent science ouverte du
CINaM

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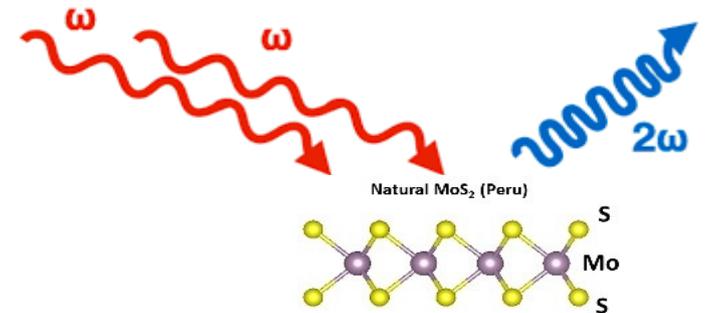
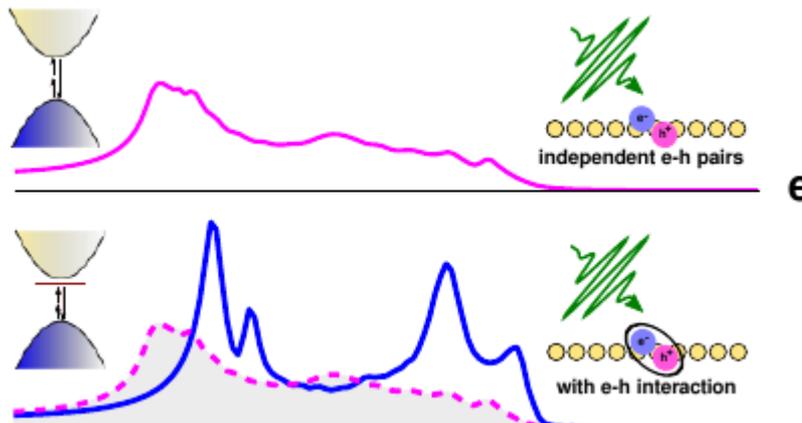
Comité scientif. GDR-HOWDI
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Code development

Yambo, Fiesta,
Turbo-RVB

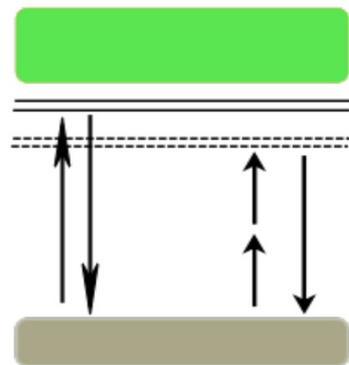
Non-linear spectroscopy

Second and third harmonic generation

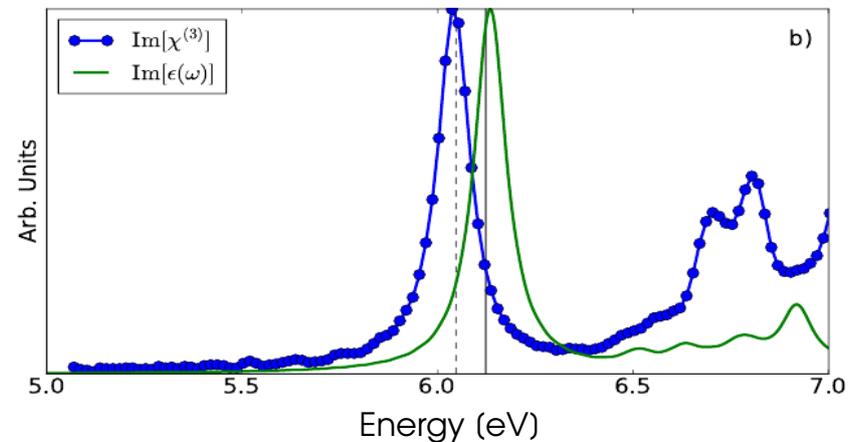


C. Attaccalite, E. Cannuccia, M. Grüning, PRB 95, 125403 (2017)
 M. Grüning, C. Attaccalite, PRB-Rapid 88, 081102 (2014)

Two-photon absorption

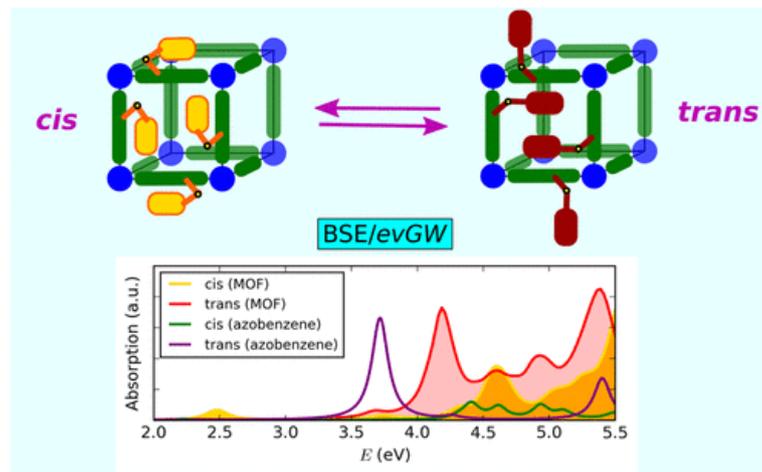
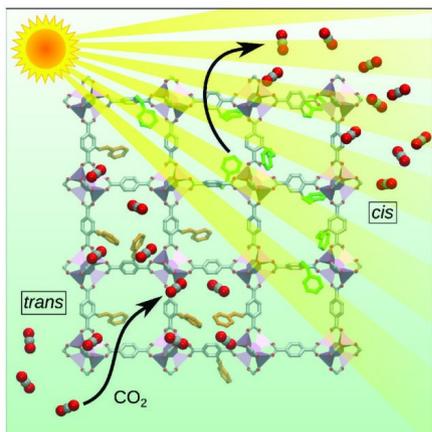


Probing dark states

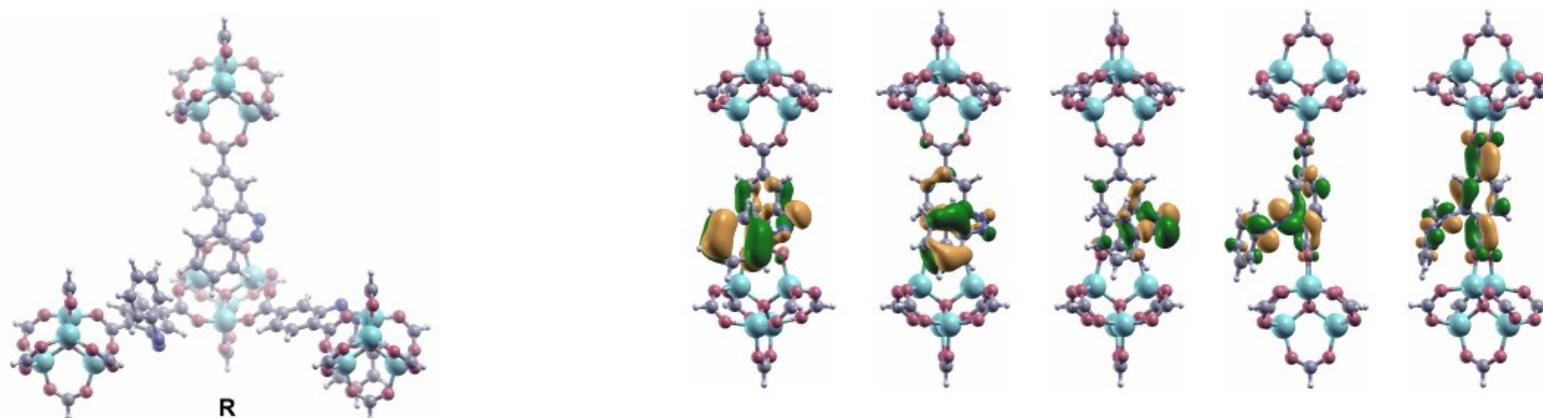


C. Attaccalite, M. Grüning, H Amara, S Latil, F Ducastelle, PRB 98 (16), 165126 (2018)

Metal organic frameworks (MOF)

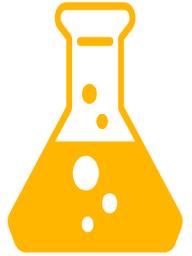


Collaboration with SIMAP (Grenoble)
financed by ANR

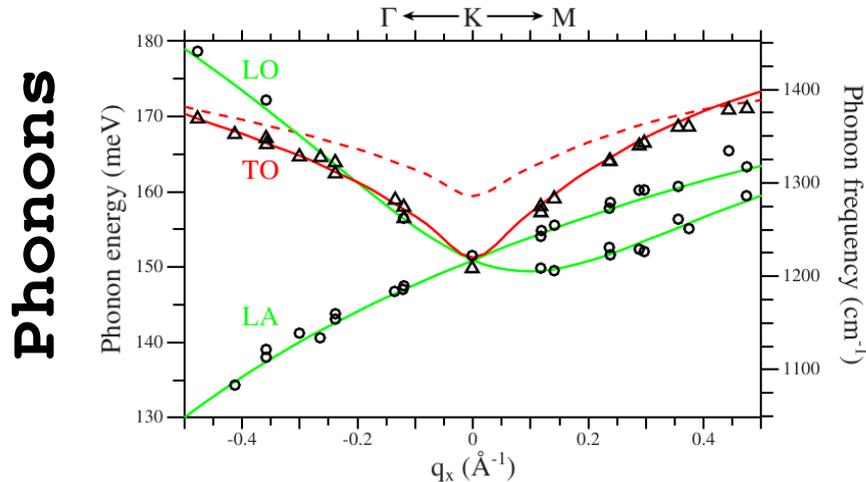


A. R. Kshirsagar, **C. Attaccalite**, X. Blase, J. Li, and R. Poloni, J. of Phys. Chem. C 125, 7401(2021)
A. R. Kshirsagar, X. Blase, **C. Attaccalite**, R. Poloni Preprint from ChemRxiv, (2021)

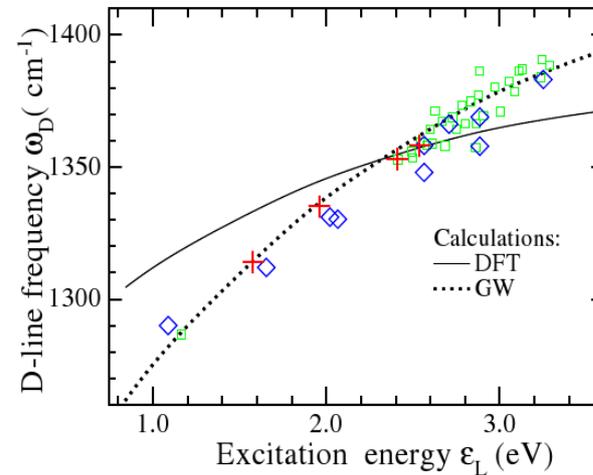
Electron **phonon** coupling



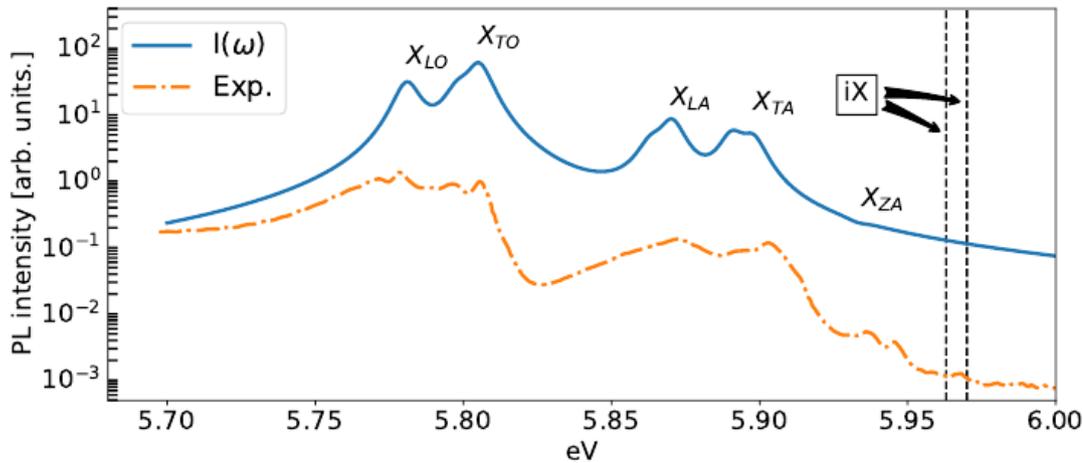
Correlation effects in the EPC



C. Attaccalite et al., *Nanoletters*, **10**, 1172(2010)

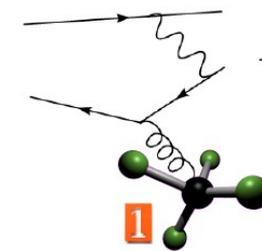


RAMAN

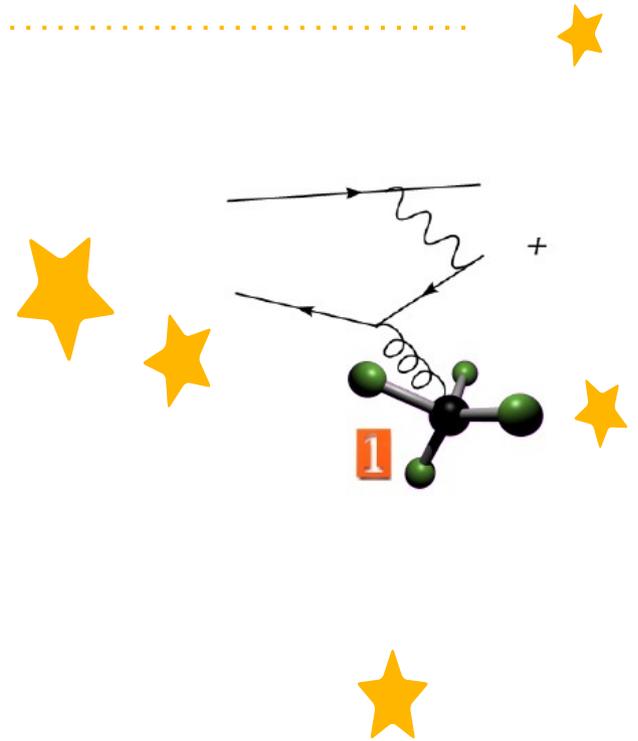


E. Cannuccia, B. Monserrat, C. Attaccalite, *PRB B* **99**, 125403 (2019)

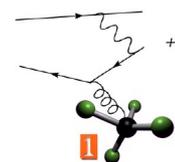
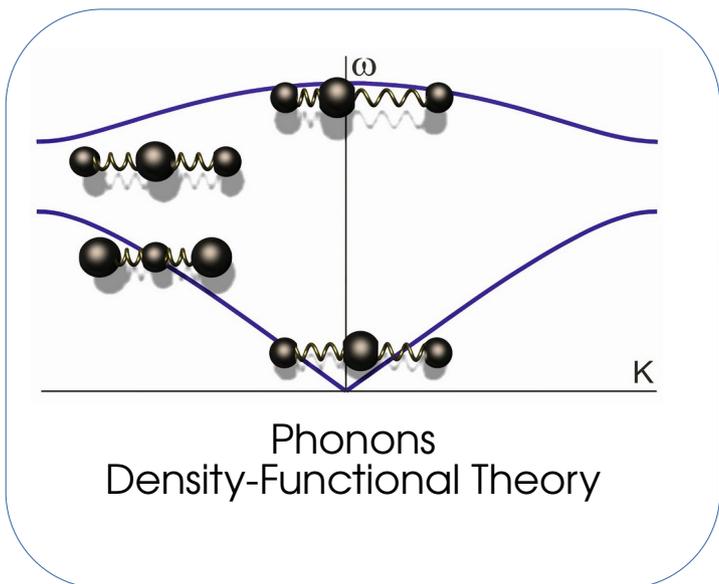
Phonon-induced luminescence



Exciton-phonon coupling from first principles

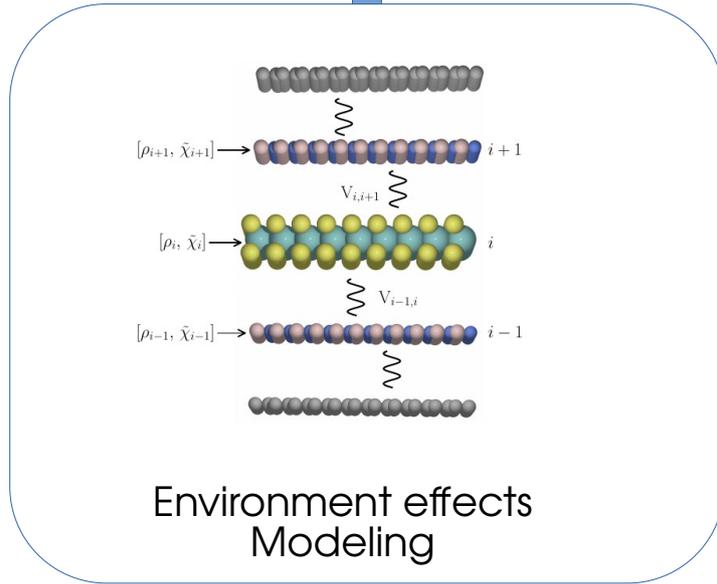
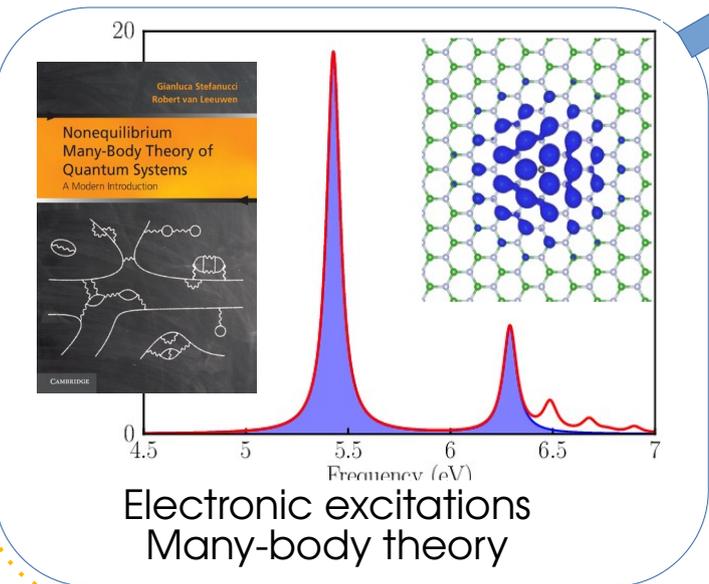


Exciton phonon coupling

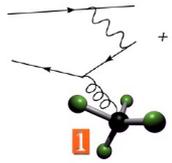
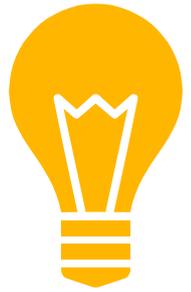


Exciton-phonon Hamiltonian

$$\mathcal{H}_{\text{el-ph}} = \sum_{kq\mu} M_{kq}^{\mu} (\mathbf{v}_{k+q}^{\dagger} \mathbf{v}_k - u_{k+q}^{\dagger} u_k) (a_{q\mu} + a_{-q\mu}^{\dagger})$$



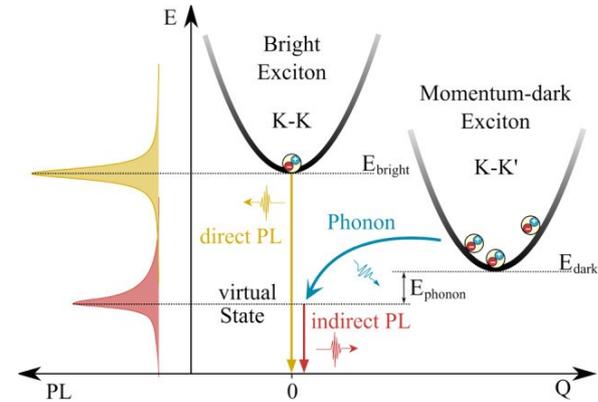
Expected results



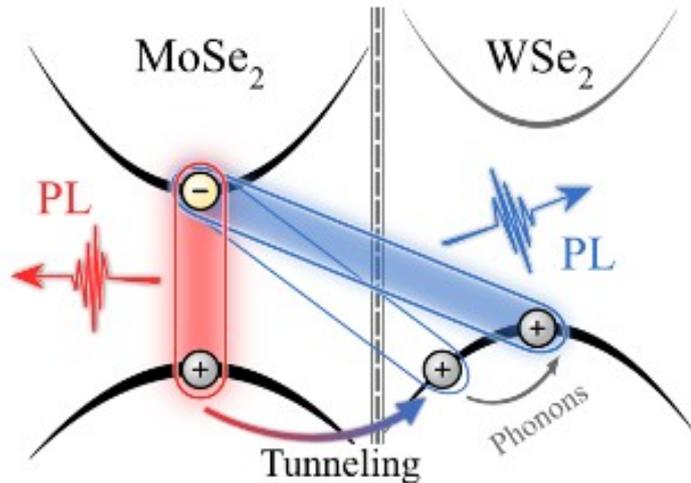
Exciton-phonon Hamiltonian

$$\mathcal{H}_{\text{el-ph}} = \sum_{kq\mu} M_{kq}^{\mu} (v_{k+q}^{\dagger} v_k - u_{k+q}^{\dagger} u_k) (a_{q\mu} + a_{-q\mu}^{\dagger})$$

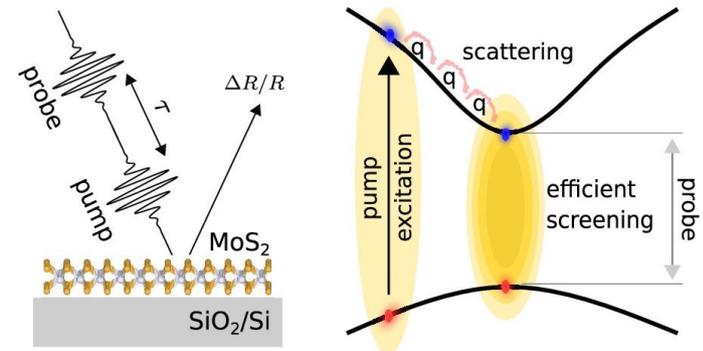
Phonon-assisted luminescence



Exciton dynamics



Pump-probe





Project

Exciton-**phonon**

from first principles

Phonon-**assisted** luminescence

Exciton-dynamics

Time-resolved **spectroscopy**

Thanks!

Any questions?

Exciton phonons



Exciton-phonon matrix elements

$$D_{S,S'}^{\lambda\mathbf{q}} = \sum_{\mathbf{k},c,v} \left[\sum_{c'} \left(A_{c'\mathbf{k}+\mathbf{q},v\mathbf{k}}^{S'(\mathbf{q})} \right)^* g_{c'\mathbf{k}+\mathbf{q},c\mathbf{k}}^{\lambda\mathbf{q}} A_{c\mathbf{k},v\mathbf{k}}^S - \sum_{v'} \left(A_{c\mathbf{k},v'\mathbf{k}-\mathbf{q}}^{S'(\mathbf{q})} \right)^* g_{v\mathbf{k},v'\mathbf{k}-\mathbf{q}}^{\lambda\mathbf{q}} A_{c\mathbf{k},v\mathbf{k}}^S \right]$$

Exciton-phonon Hamiltonian

$$H^{exc-ph} = \sum_{S,\mathbf{Q}} E_{\mathbf{Q}}^S a_{S\mathbf{Q}}^\dagger a_{S\mathbf{Q}} + \sum_{\lambda\mathbf{q}} \omega_{\lambda\mathbf{q}} b_{\lambda\mathbf{q}}^\dagger b_{\lambda\mathbf{q}} + \sum_{S,S',\mathbf{Q},\mathbf{q}} D_{S,S'}^{\lambda\mathbf{q}}(\mathbf{Q}) a_{S\mathbf{Q}+\mathbf{q}}^\dagger a_{S'\mathbf{Q}} (b_{\lambda\mathbf{q}} + b_{\lambda,-\mathbf{q}}^\dagger)$$

Equations of motion

$$\frac{d}{dt} n_{\mathbf{k}} = \frac{2}{\hbar} \Im \{ M_{\mathbf{k}} S_{\mathbf{k}} \},$$

Phonon occupation

$$i\hbar \frac{d}{dt} S_{\mathbf{k}} = (E_0 - \omega_{\mathbf{k}}) S_{\mathbf{k}} - M_{\mathbf{k}}^* N_0 + \sum_{\mathbf{q},\zeta=\pm} D_{\mathbf{q}} \mathcal{U}_{\mathbf{k}\mathbf{q}}^\zeta + \sum_{\mathbf{k}'} M_{\mathbf{k}'}^* n_{\mathbf{k}\mathbf{k}'} \quad \text{Polarization}$$

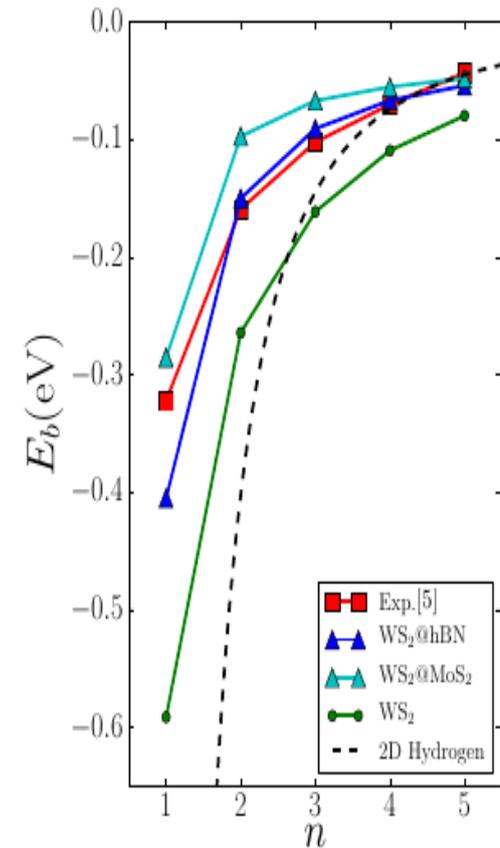
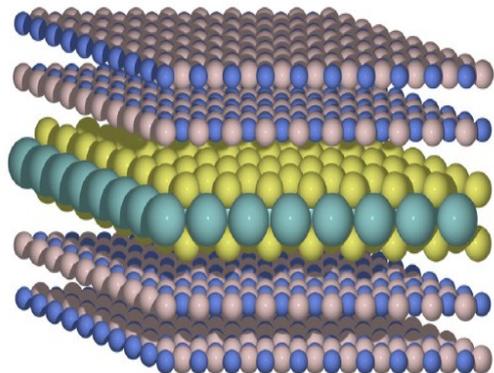
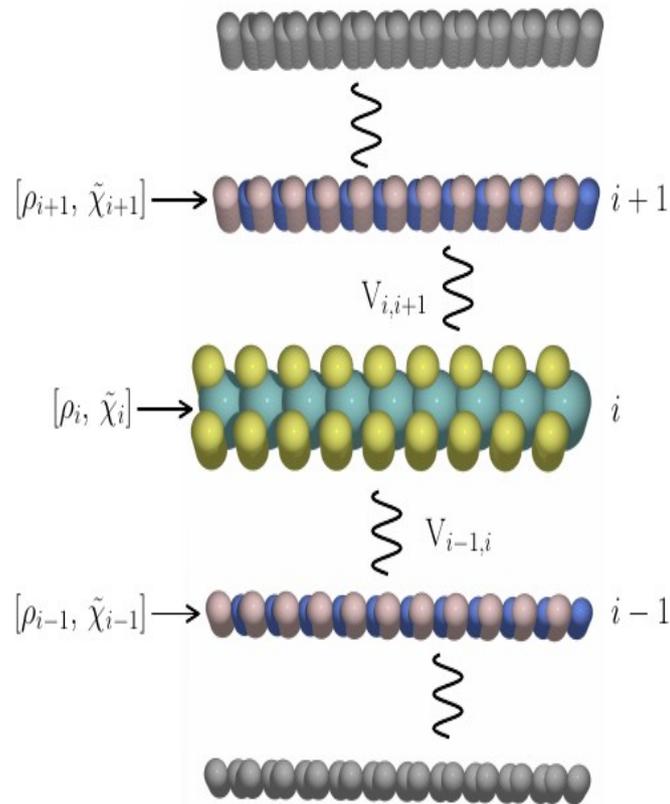
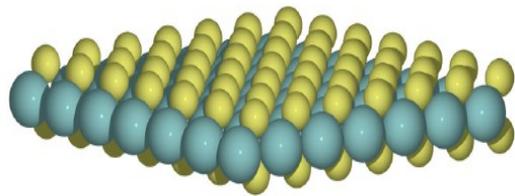
$$i\hbar \frac{d}{dt} \mathcal{U}_{\mathbf{k}\mathbf{q}}^\zeta = (E_{-\mathbf{q}} - \zeta \Omega_{\mathbf{q}} - \omega_{\mathbf{k}}) \mathcal{U}_{\mathbf{k}\mathbf{q}}^\zeta - M_{\mathbf{k}}^* C_{0\mathbf{q}}^\zeta + D_{\mathbf{q}}^* \eta_{\mathbf{q}}^\zeta S_{\mathbf{k}} + \sum_{\mathbf{q}',\zeta'=\pm} D_{\mathbf{q}'} X_{\mathbf{k}\mathbf{q}\mathbf{q}'}^{\zeta\zeta'}, \quad \text{PH-assist. pol.}$$

$$i\hbar \frac{d}{dt} C_{\mathbf{Q}\mathbf{q}}^\zeta = (E_{\mathbf{Q}-\mathbf{q}} - \zeta \Omega_{\mathbf{q}} - E_{\mathbf{Q}}) C_{\mathbf{Q}\mathbf{q}}^\zeta - D_{\mathbf{q}}^* Q_{\mathbf{Q}\mathbf{q}}^\zeta \quad \text{Exciton-phonon}$$

$$- \sum_{\mathbf{k}} (M_{\mathbf{k}} \mathcal{U}_{\mathbf{k}\mathbf{q}}^\zeta \delta_{\mathbf{Q},0} - M_{\mathbf{k}}^* \mathcal{U}_{\mathbf{k},-\mathbf{q}}^{-\zeta} \delta_{\mathbf{Q},-\mathbf{q}}) + \sum_{\mathbf{q}',\zeta'=\pm} (D_{\mathbf{q}'} Y_{\mathbf{Q}\mathbf{q}\mathbf{q}'}^{\zeta\zeta'} - D_{\mathbf{q}'}^* Y_{\mathbf{Q}+\mathbf{q}',\mathbf{q},-\mathbf{q}'}^{\zeta\zeta'}),$$

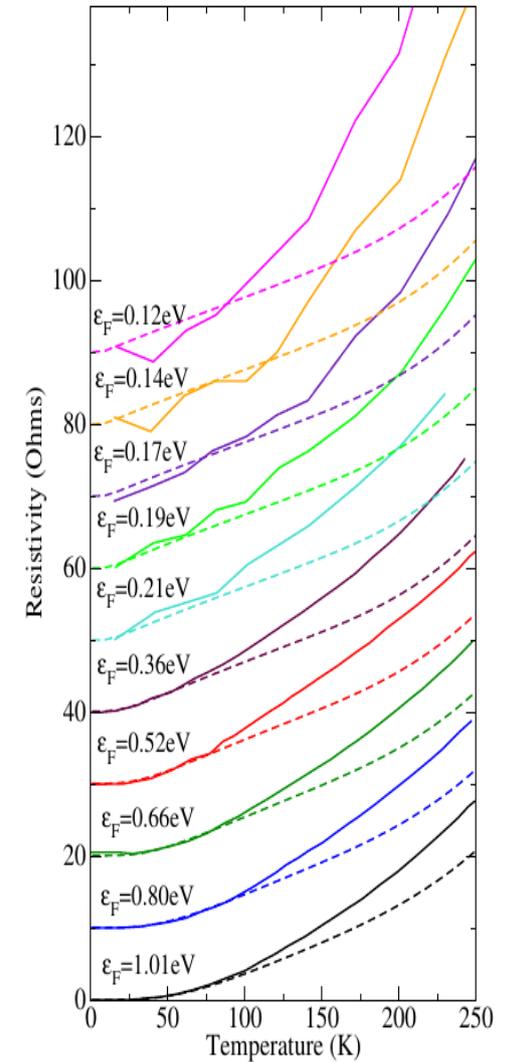
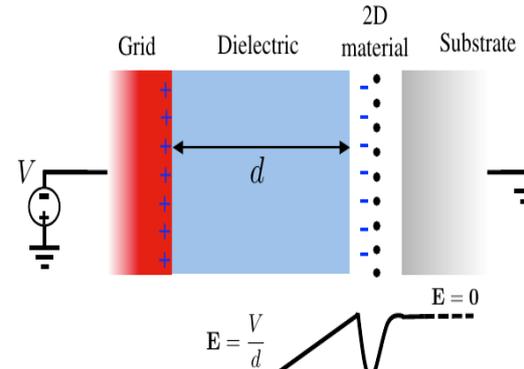
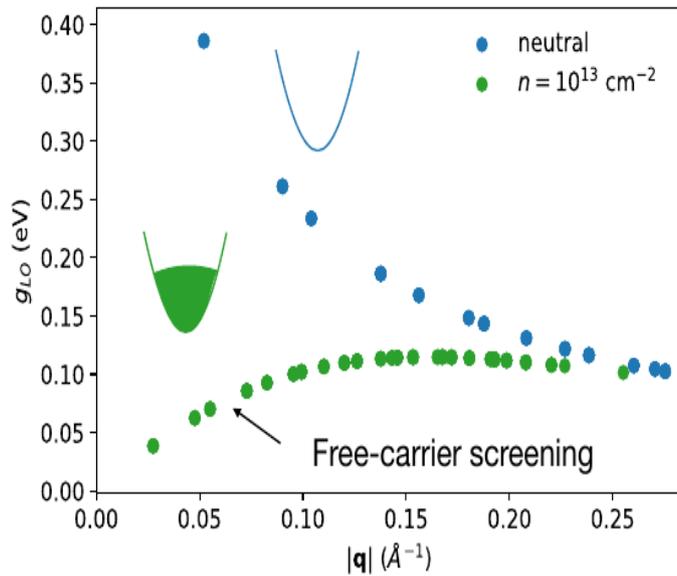
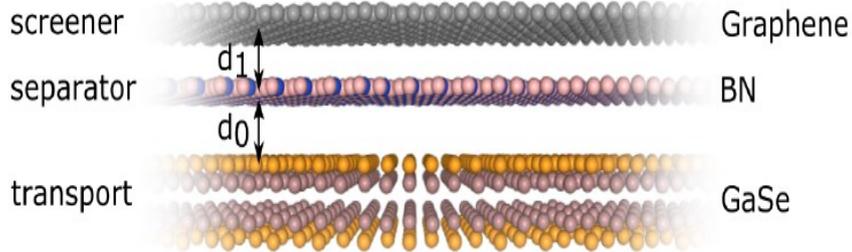
$$\frac{d}{dt} N_{\mathbf{Q}} = -\frac{2}{\hbar} \sum_{\mathbf{k}} \Im \{ M_{\mathbf{k}} S_{\mathbf{k}} \} \delta_{\mathbf{Q},0} - \frac{i}{\hbar} \sum_{\mathbf{q},\zeta=\pm} D_{\mathbf{q}} (C_{\mathbf{Q}\mathbf{q}}^\zeta - C_{\mathbf{Q}+\mathbf{q},-\mathbf{q}}^\zeta) \quad \text{Exciton-density}$$

Quantum Electrostatic Heterostructure model and its relatives



K. Andersen, S. Latini and K.S. Thygesen, *Nanoletter*, **15**, 4616 (2015)
 L. Sponza, F. Ducastelle, <https://arxiv.org/abs/2011.07811>

Environment: phonons



T. Sohler, et al. Phys. Rev. Mat. 5, 024004 (2021)