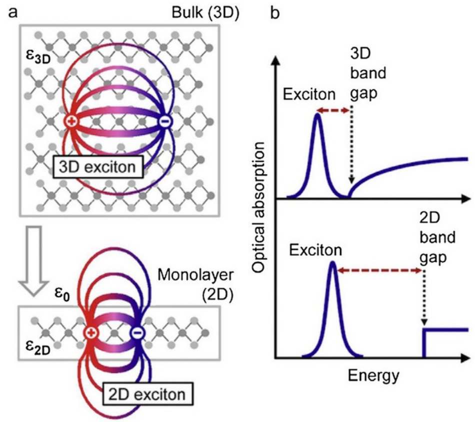
Axis 3 : Optical, excitonic and photonic properties

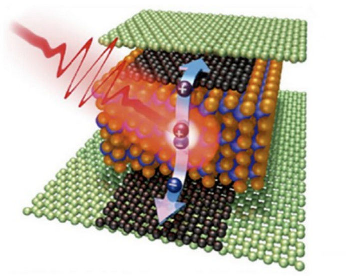
Recent theoretical developments for 2D heterostructures



Claudio Attaccalite
Aix-Marseille Univ./CNRS

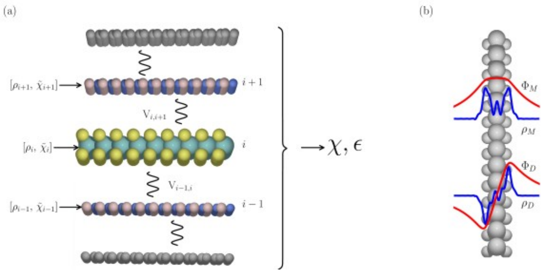
GDR HOWDI : annual meeting, March 2021

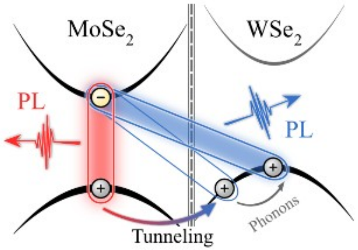
Recent theoretical developments for optical properties in heterostructures



1) Optical excitation in complex structures

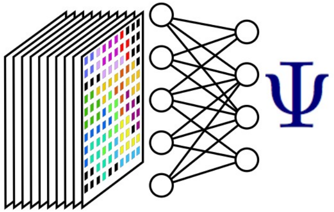
2) Environment effects





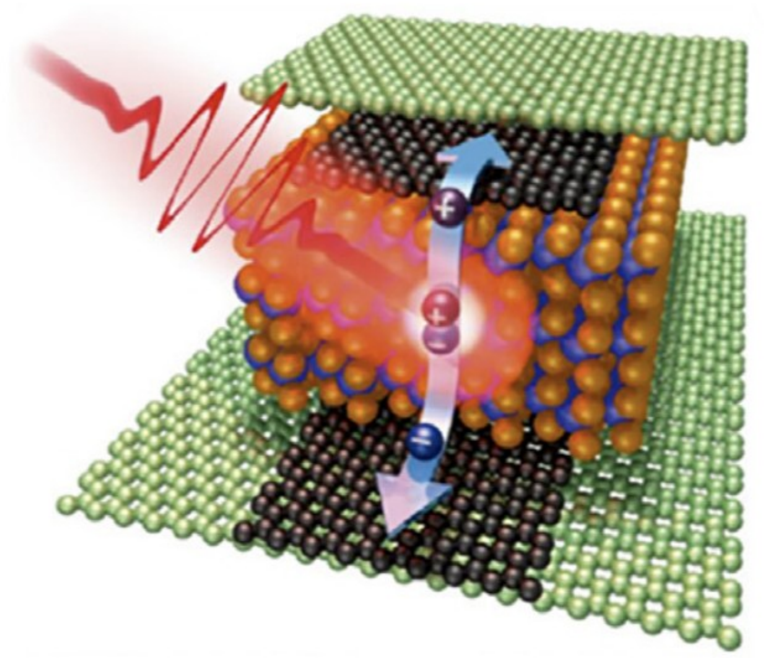
3) Excitations dynamics

4) Machine learning for heterostructures



Axis 3 : Optical, excitonic and photonic properties

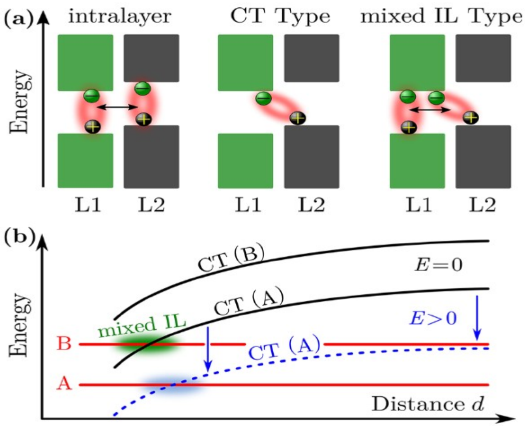
1) Optical excitation in complex structures

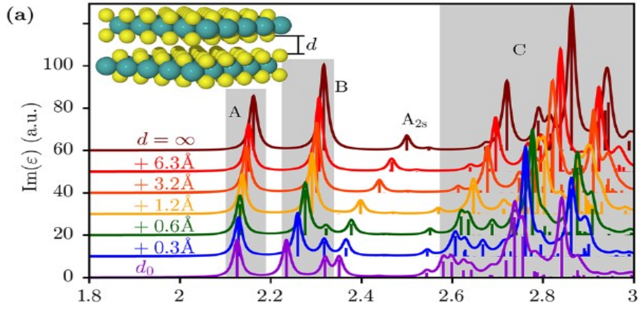


Axis 3 : Optical, excitonic and photonic properties

Optical excitations in hetereostructures

Intra/inter layer excitons

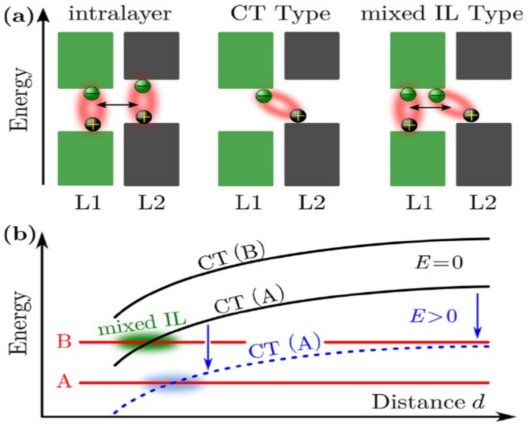


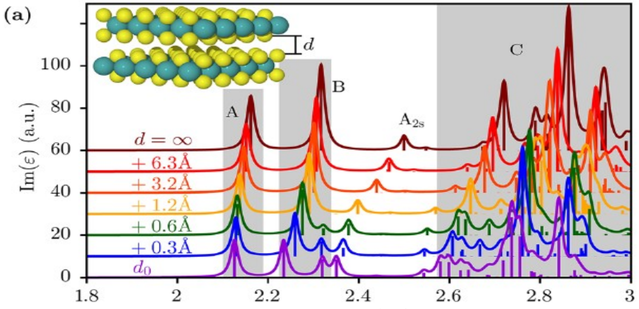


T. Deilmann et al. Nanoletters **18**, 2984(2018)

Optical excitations in hetereostructures

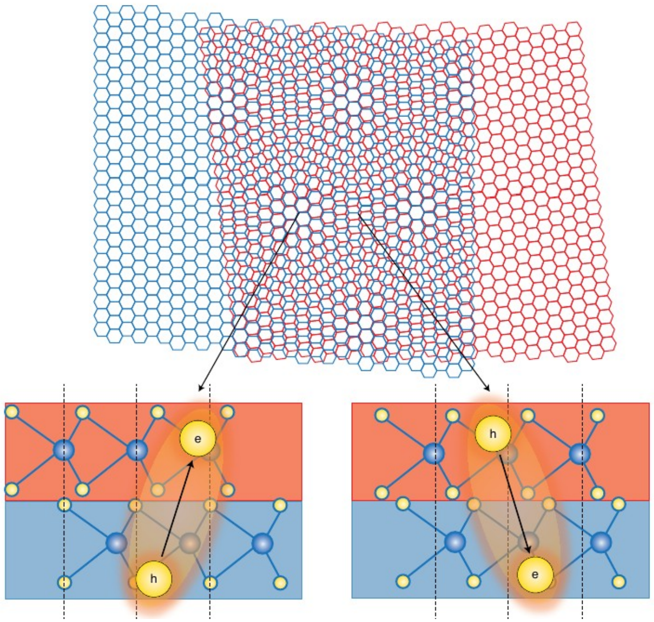
Intra/inter layer excitons





T. Deilmann et al. Nanoletters **18**, 2984(2018)

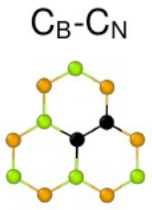
Twisted materials

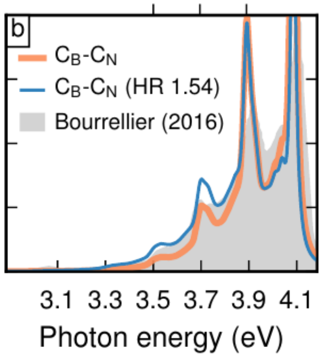


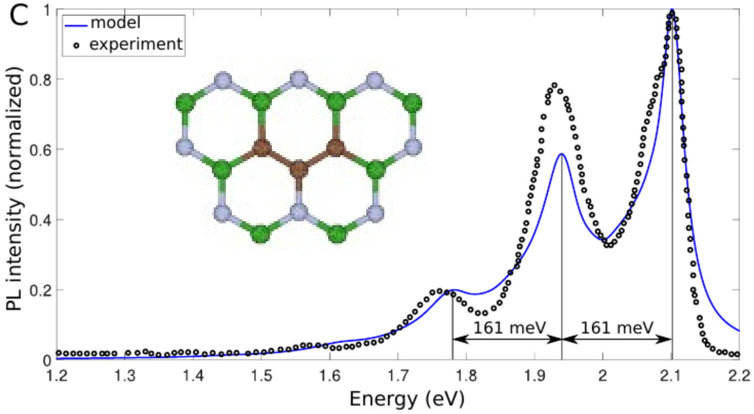
Nature Nanotech. **15**, 726 (2020)

Scattering with defects

Defects identification using vibrational modes







C. Linderälv, et al. arxiv.org/abs/2008.05817
C. Jara et al, arxiv.org/abs/2007.15990

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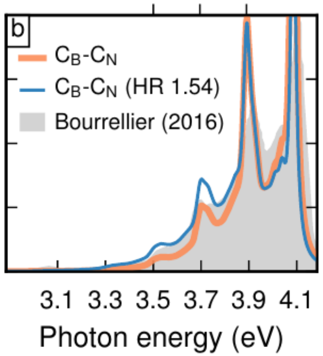
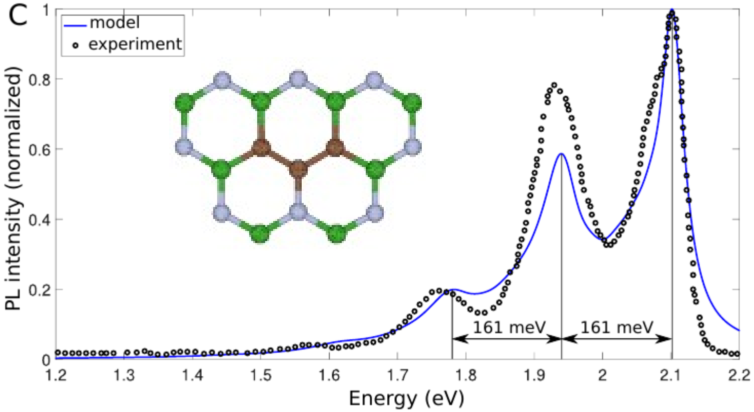
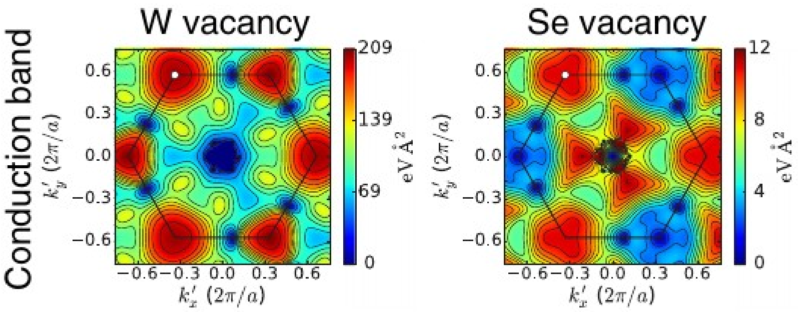
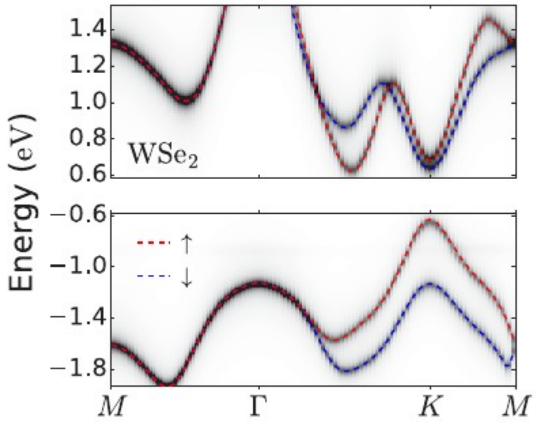




C. Linderälv, et al. arxiv.org/abs/2008.05817
C. Jara et al, arxiv.org/abs/2007.15990

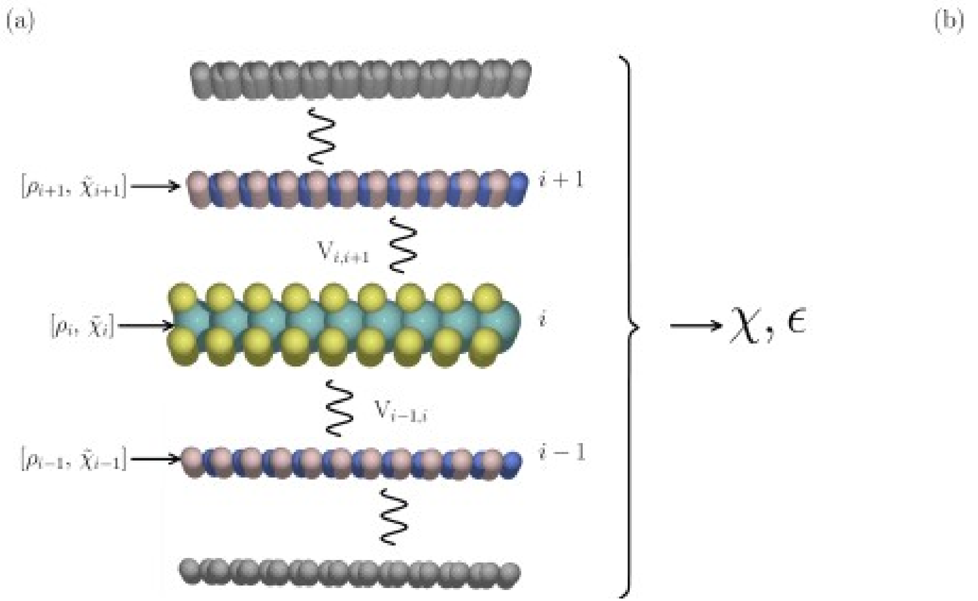
Spectral properties of defects





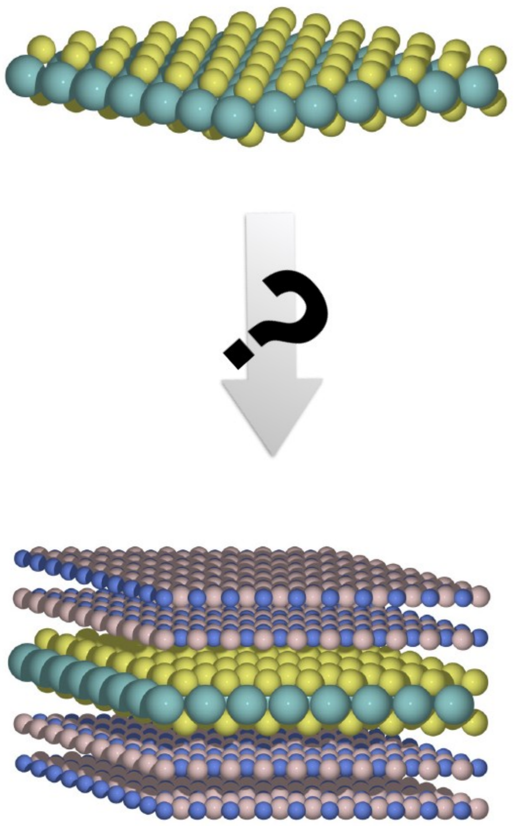
K. Kaasbjerg Phys. Rev. B **101**, 045433(2020)

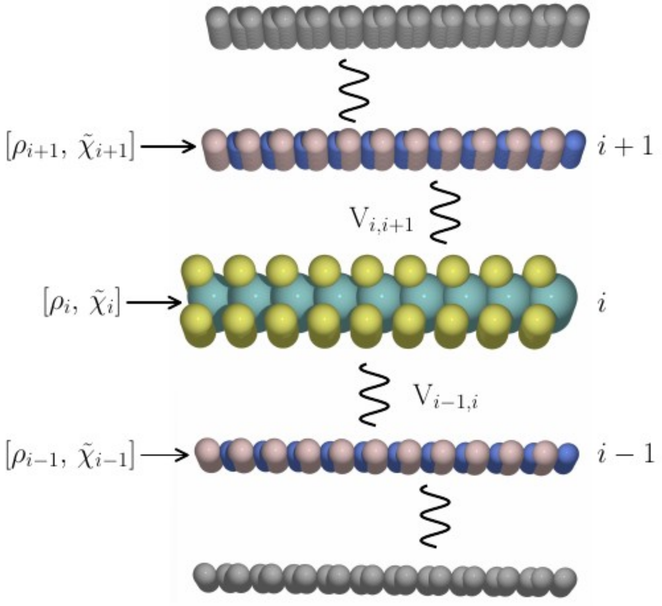
2) Environment effects

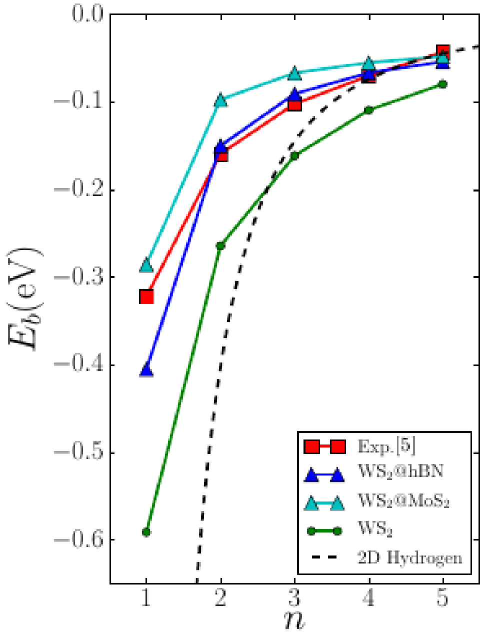


Axis 3 : Optical, excitonic and photonic properties

Quantum Electrostatic Heterostructure model and its relatives

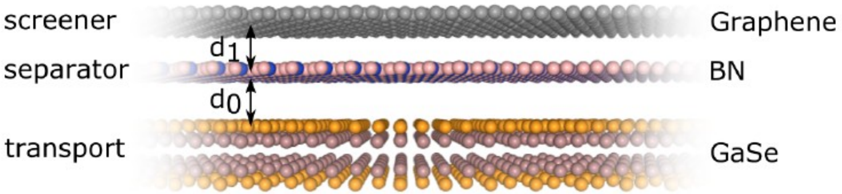


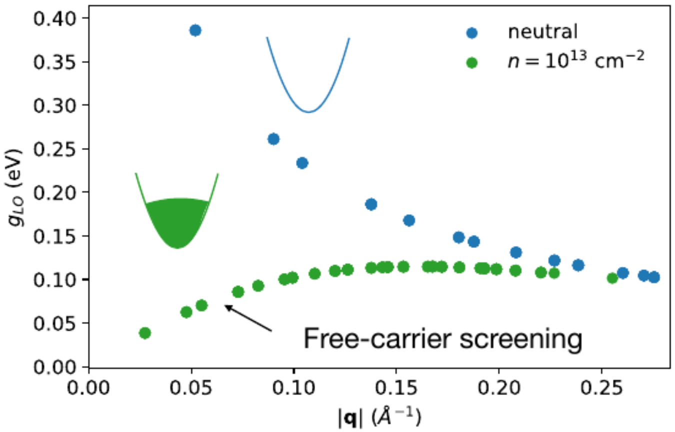




K. Andersen, S. Latini and K.S. Thygesen, Nanoletter, **15**, 4616 (2015)
L. Sponza, F. Ducastelle, https://arxiv.org/abs/2011.07811

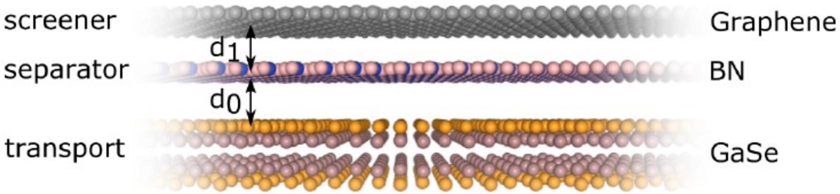
Environment: phonons

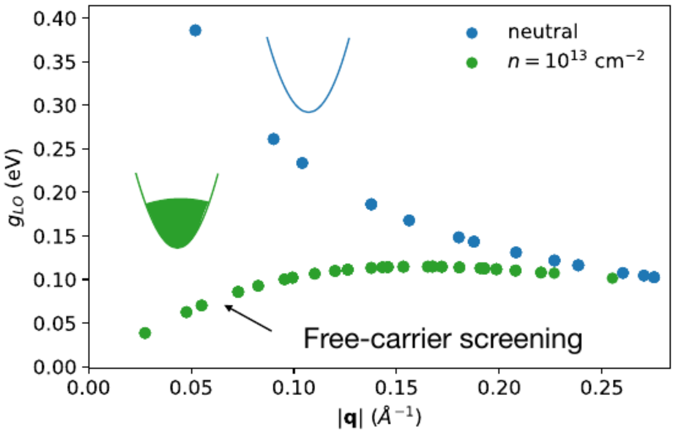




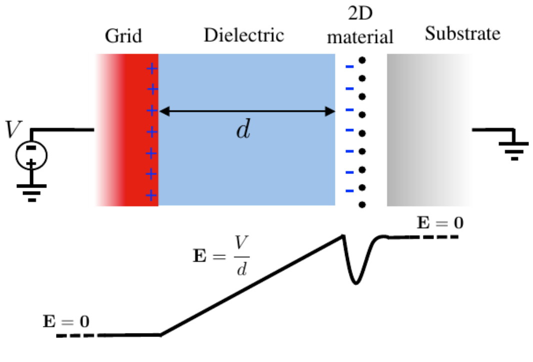
T. Sohier, et al. Phys. Rev. Mat. **5**, 024004 (2021)

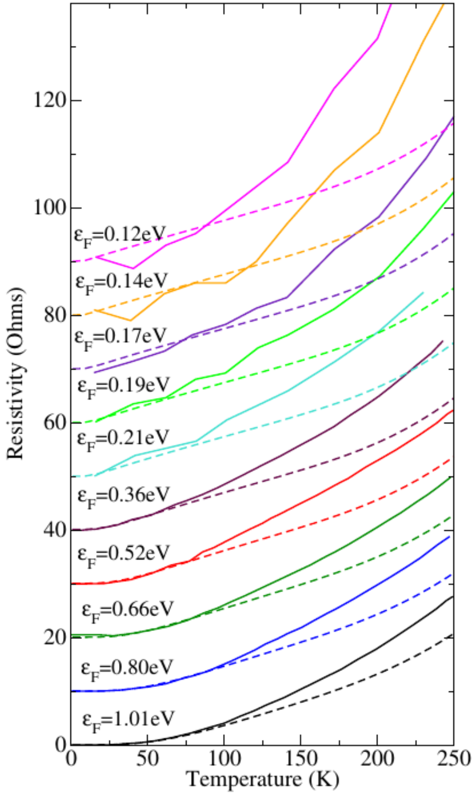
Environment: phonons



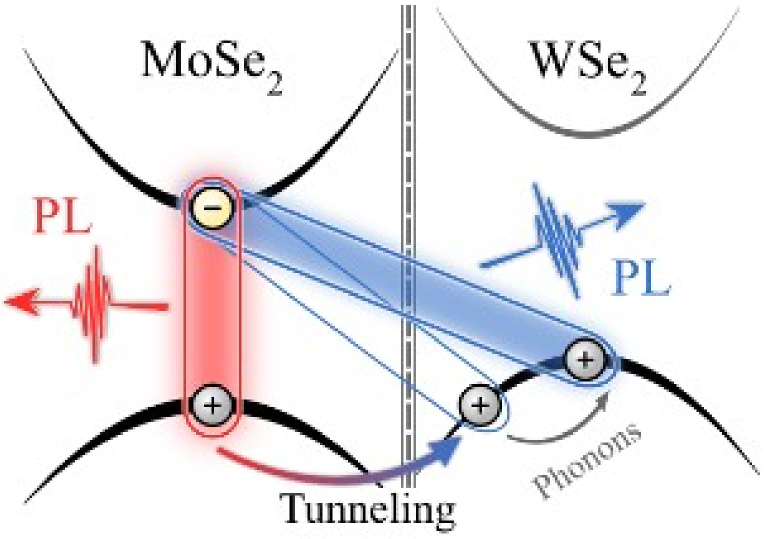


T. Sohier, et al. Phys. Rev. Mat. **5**, 024004 (2021)

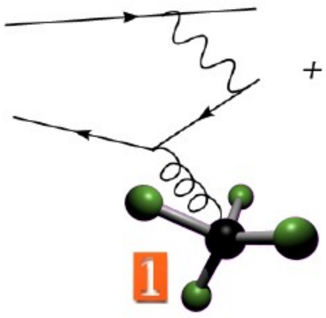




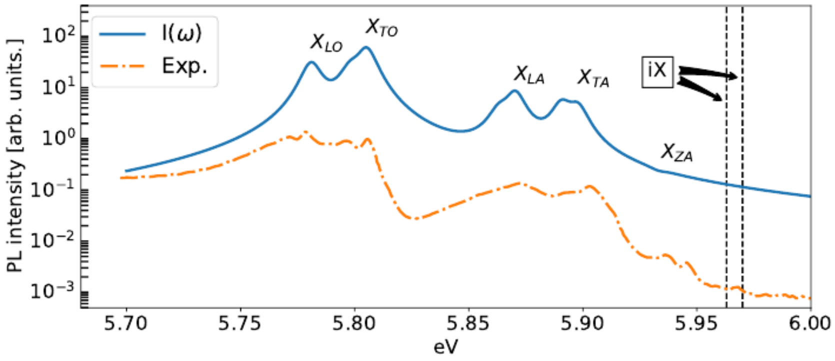
2) Excitations dynamics



Coupling excitons and phonons

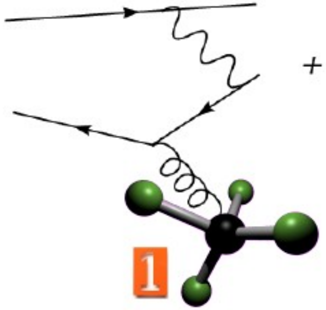


Phonon-assisted luminescence (hBN)



E Cannuccia,et al. Rev. B **99**, 081109(R) (2019)
F. Paleari, et al., Phys. Rev. Lett. **122**, 187401
G. Cassabois et al., Nature Photonics, **10**, 262 (2016)

Coupling excitons and phonons



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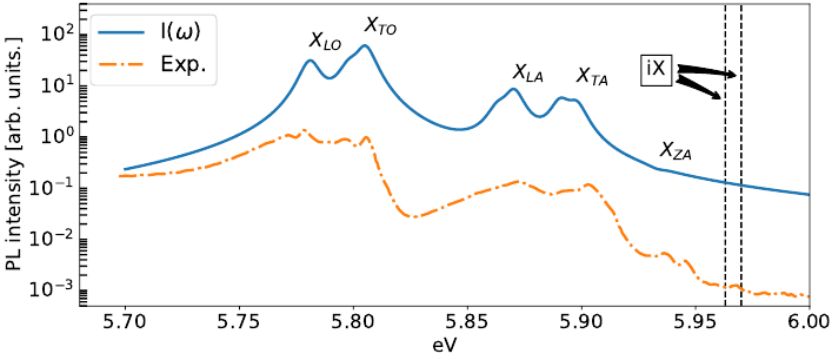
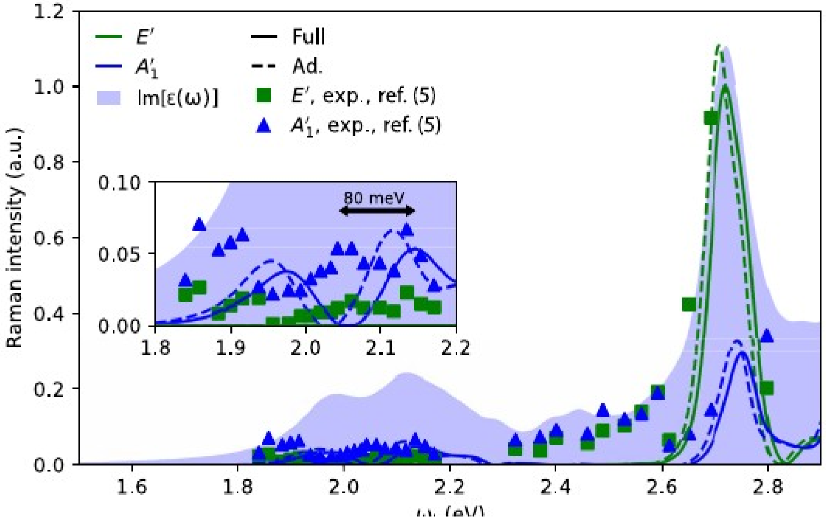




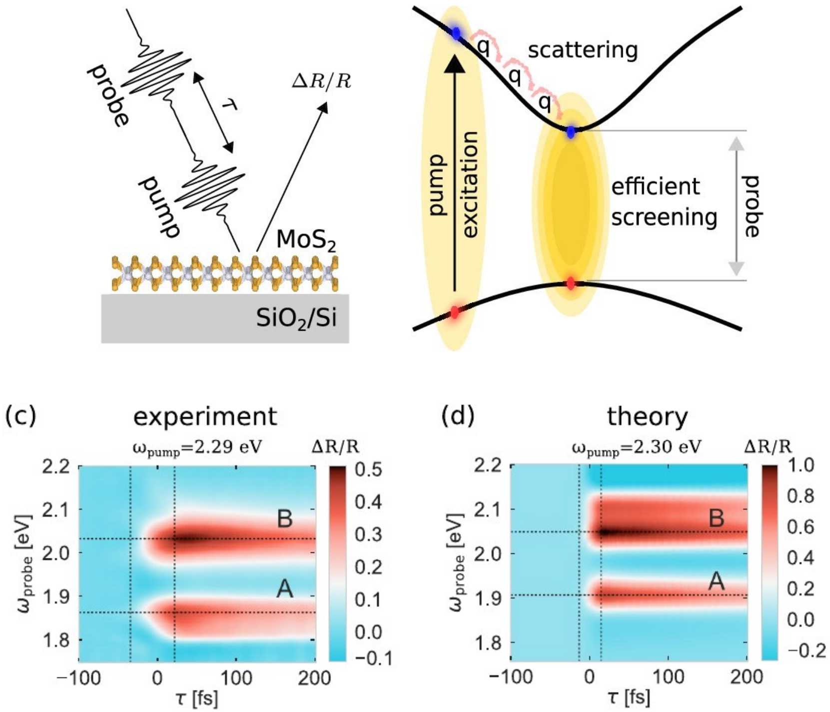
Non-adiabatic exciton-phonon coupling in Raman (MoS2)

E Cannuccia,et al. Rev. B **99**, 081109(R) (2019)
F. Paleari, et al., Phys. Rev. Lett. **122**, 187401
G. Cassabois et al., Nature Photonics, **10**, 262 (2016)

S. Reichardt and L. Wirtz Sci. Adv. 2020; 6 (202)

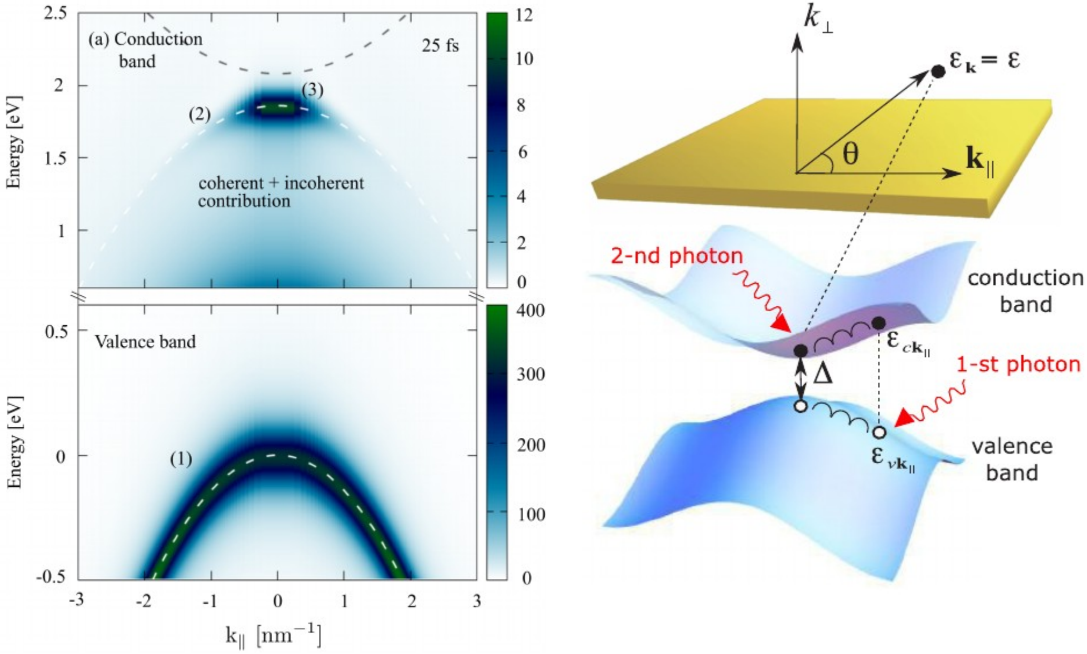
Real-time dynamics

Pump and probe



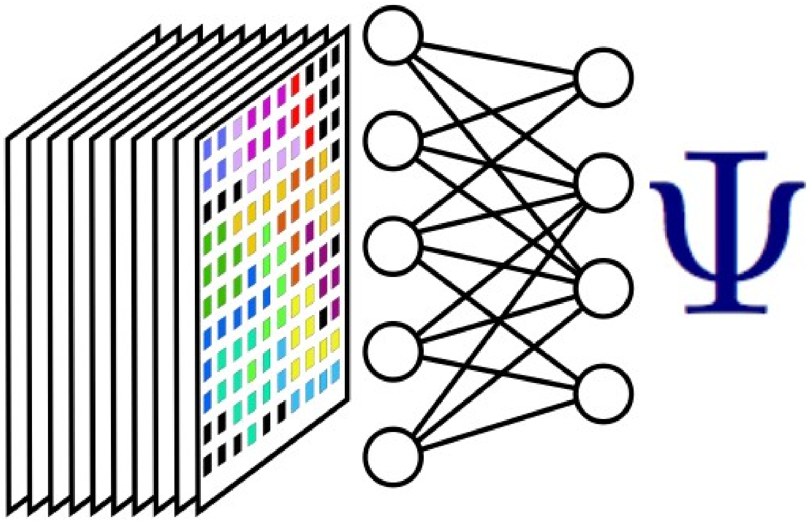
V. Smejkal et al. ACS Nano, **15**, 1, 1179 (2021)

Time-resolved ARPES



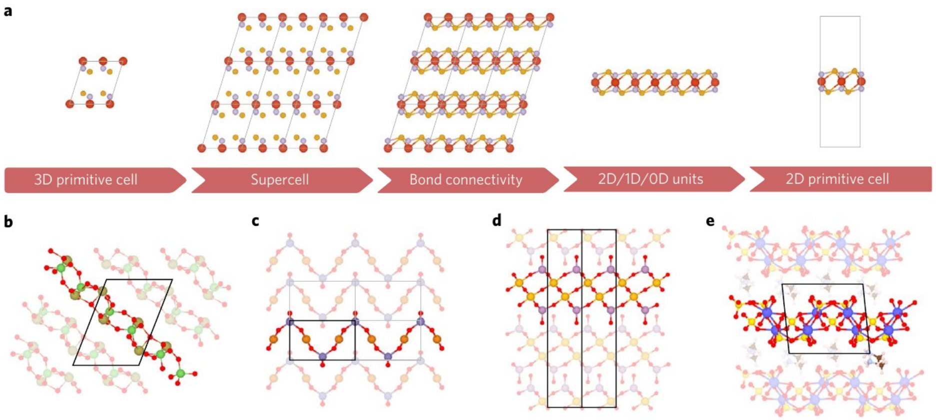
E. Perfetto, Phys. Rev. B, **94**, 245303 (2020)
D. Christiansen, et al. Phys. Rev. B **100**, 205401(2019)

4) Machine learning for heterostructures

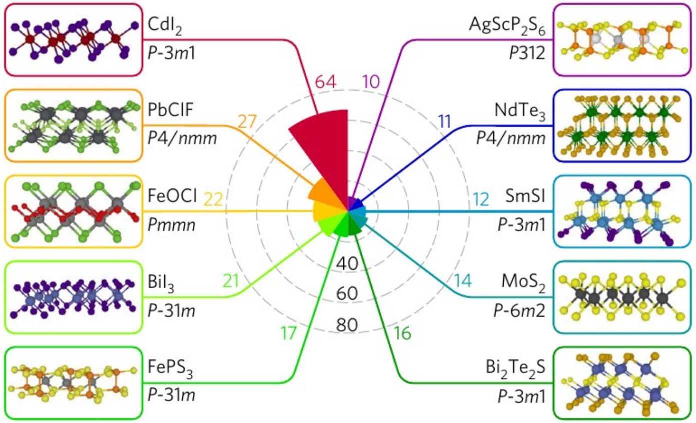


Axis 3 : Optical, excitonic and photonic properties

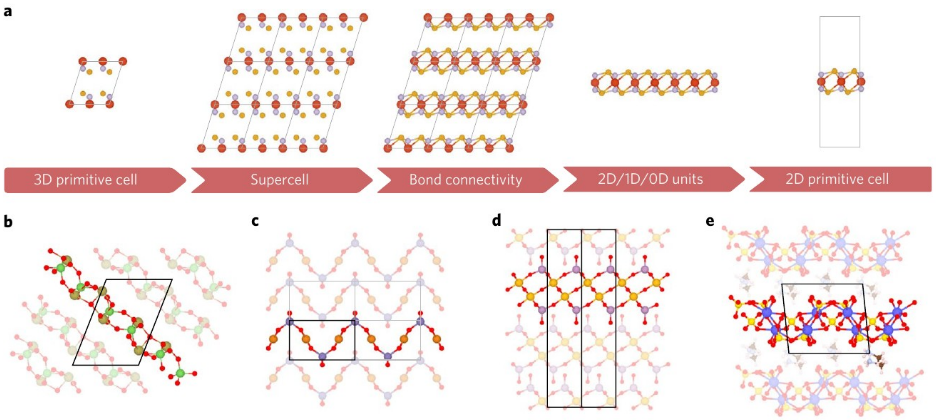
Machine learning for 2D materials



New easily exfoliable 2D materials



Machine learning for 2D materials



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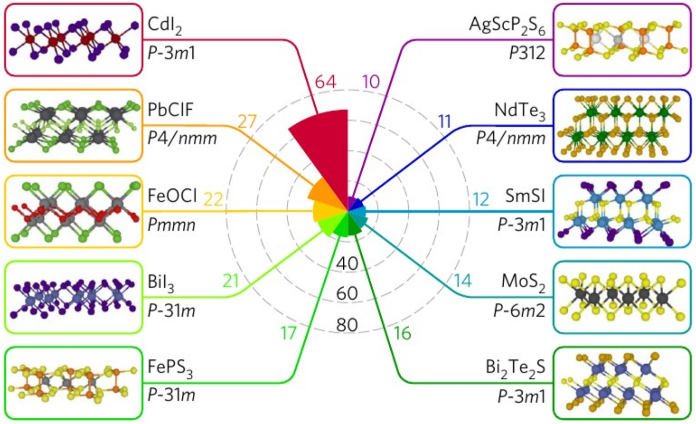
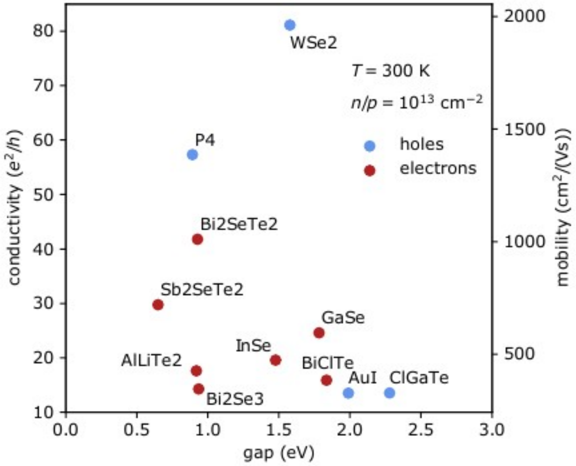


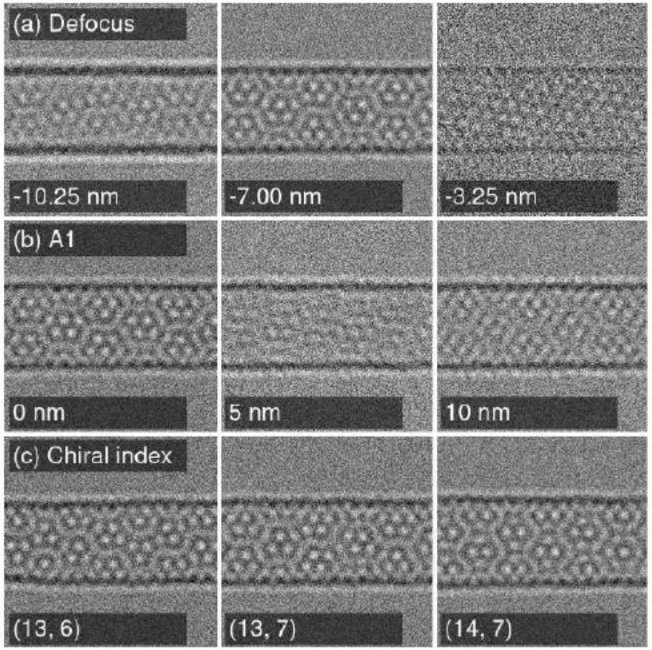
Novel high-conductivity 2D semiconductors

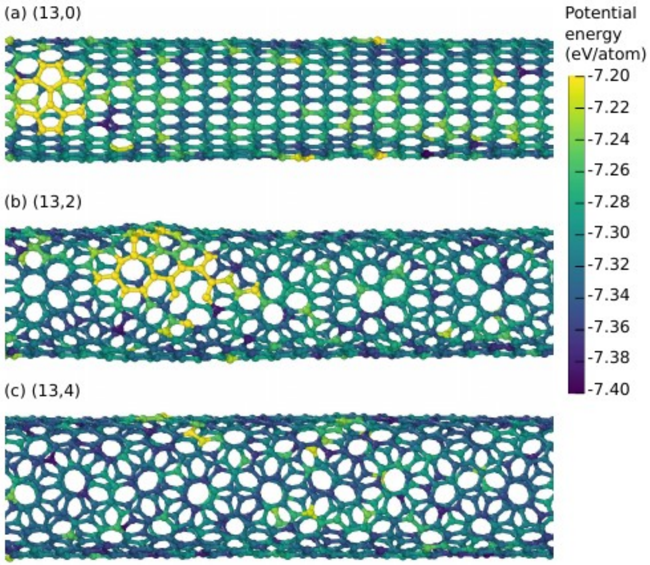


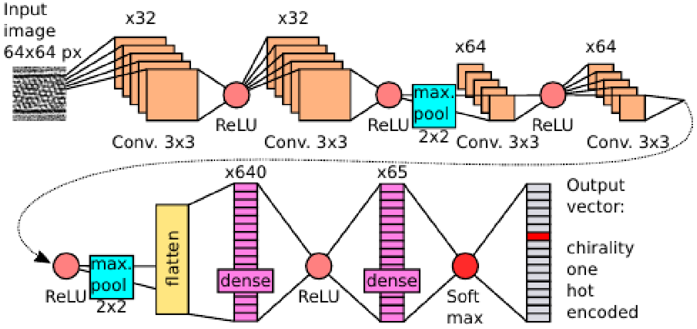
N. Mounet et al. Nature Nanotech.,**13**, 246 (2018)
T. Sohier et al. 2D Materials, **8**, 015025 (2021)

Machine learning for experiment analysis

Determining the chiral indices from high-resolution transmission electron microscopy analysis





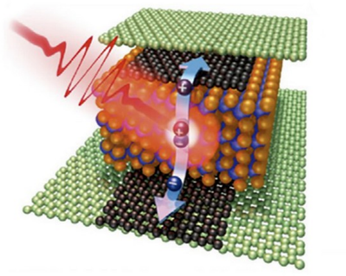


G.D. Forster et al. Carbon **169**, 465 (2020)

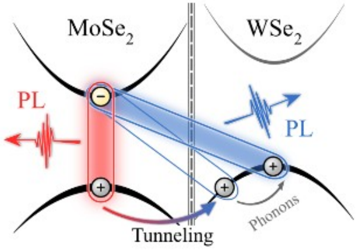
Axis 3 : Optical, excitonic and photonic properties

Merci pour votre attention

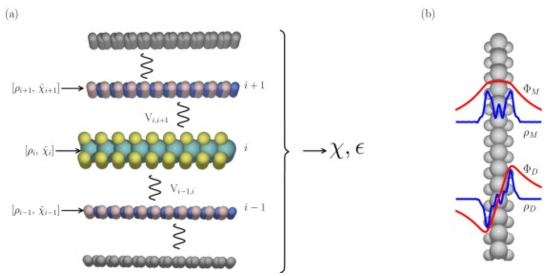
Structure



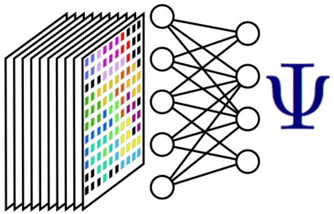
Dynamics



Environment



Machine learning



GDR HOWDI : annual meeting, March 2021