GRAPHENE AND 2DM VIRTUAL CONFERENCE & EXPO

Graphene online 2020 October 19-23

Thermal transport modelling through van der Waals heterostructures [1]

Sara Fiore Mathieu Luisier

Integrated Systems Laboratory, ETH Zurich, 8092 Zurich, Switzerland

Goal

Engineer the heat flow through nanostructures combining Transistion Metal Dichalcogenide (TMD) monolayers with different geometries through *ab initio* simulations of ballistic quantum thermal transport

Transport Equations

DFT

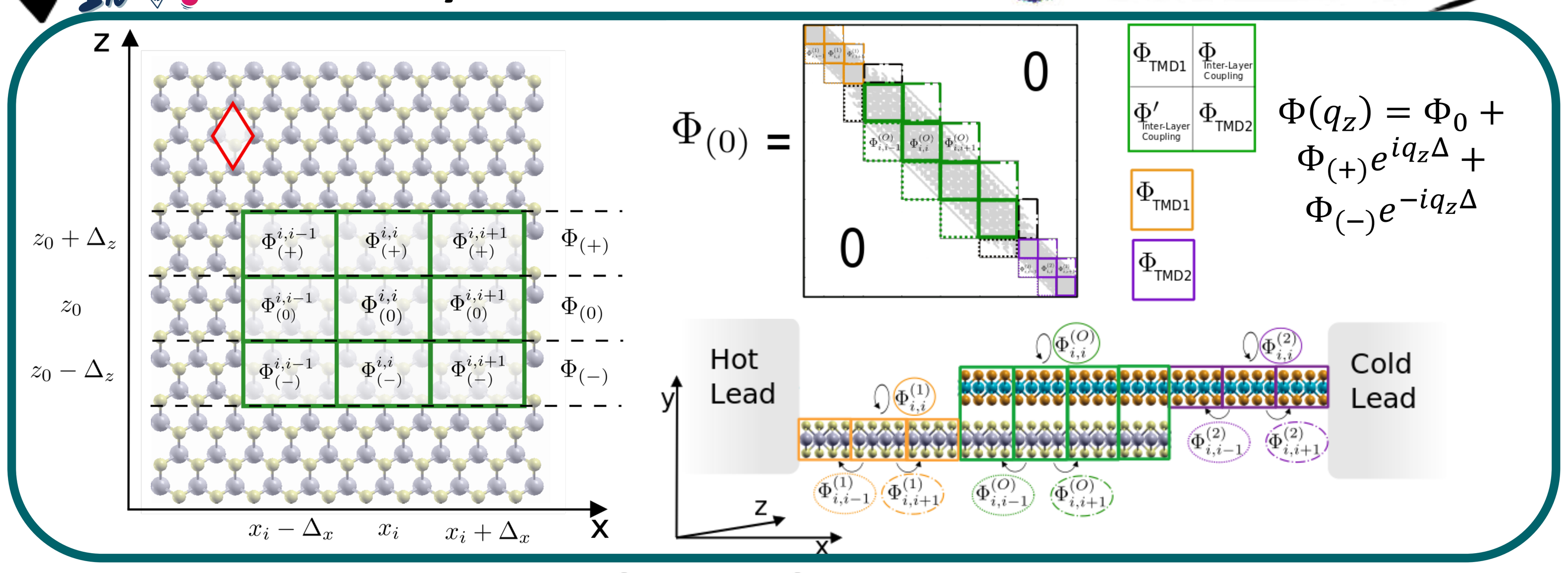
Φ_{DFT}, ω

$$(\omega^2\mathbb{I} - \Phi - \Pi^{RB})\varphi = Inj$$

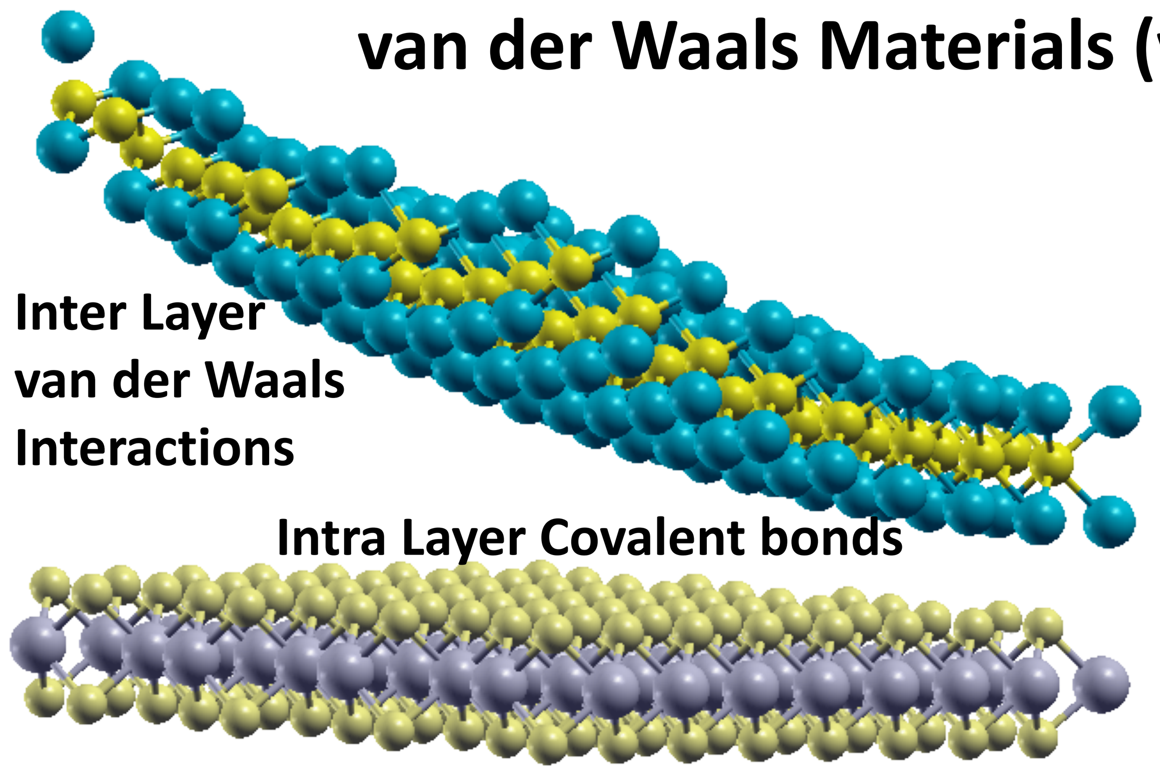
$$I_{Th} = \sum_{q_z} \frac{1}{N_{q_z}} \int \frac{d\omega}{2\pi} \mathcal{T}(\hbar\omega, q_z)(\hbar\omega)(b(T_L,\hbar\omega) - b(T_R,\hbar\omega))$$

OMEN

Device Dynamical Matrix



van der Waals Materials (vdWM)



Promising Applications
- Vertical FET (electronics)
- Photodiodes (optoelectronic)
- Spin FET (spintronic)
- ...

New Features
with respect to their constituents
- Band alignment
- Fast charge transport
- Inter-layer excitons
- ...

Materials Selection Criteria

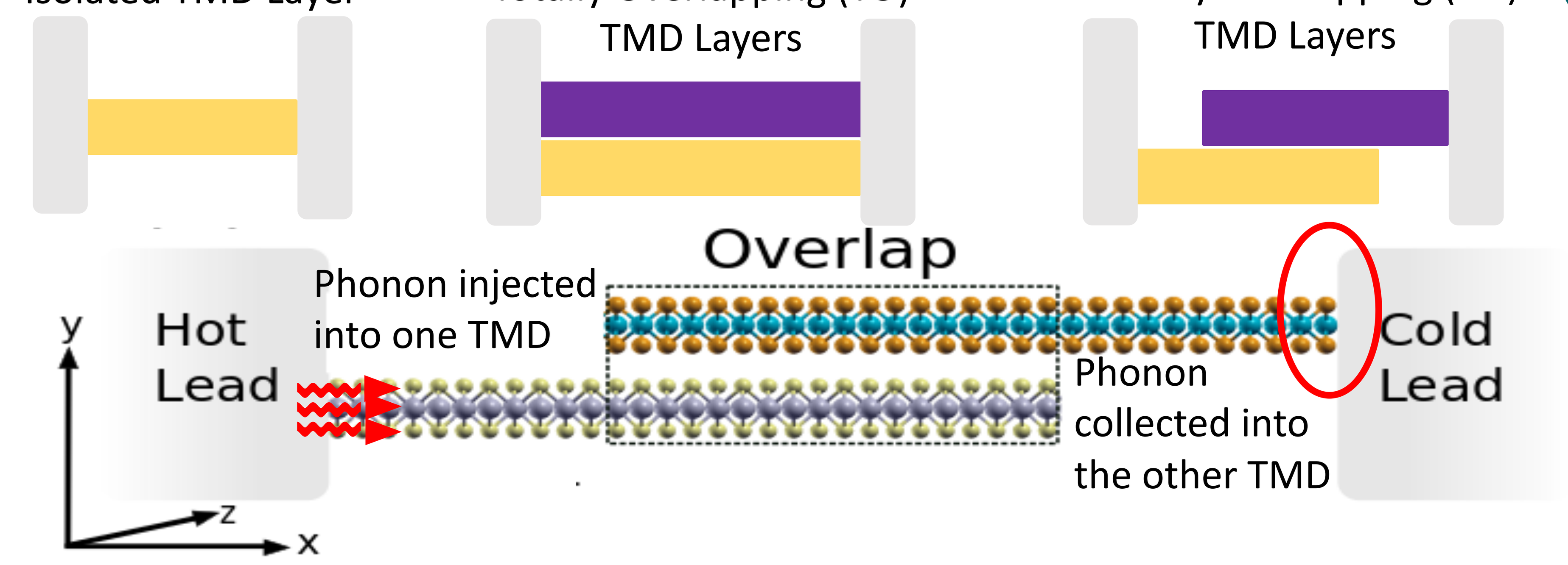
	✓	✗
Common cell	N = N1 + N2	supercell
Atomic positions	unchanged	changed
Lattice	2H	1T'

Transition Metals : Mo, W

Chalcogenides : S, Se, Te

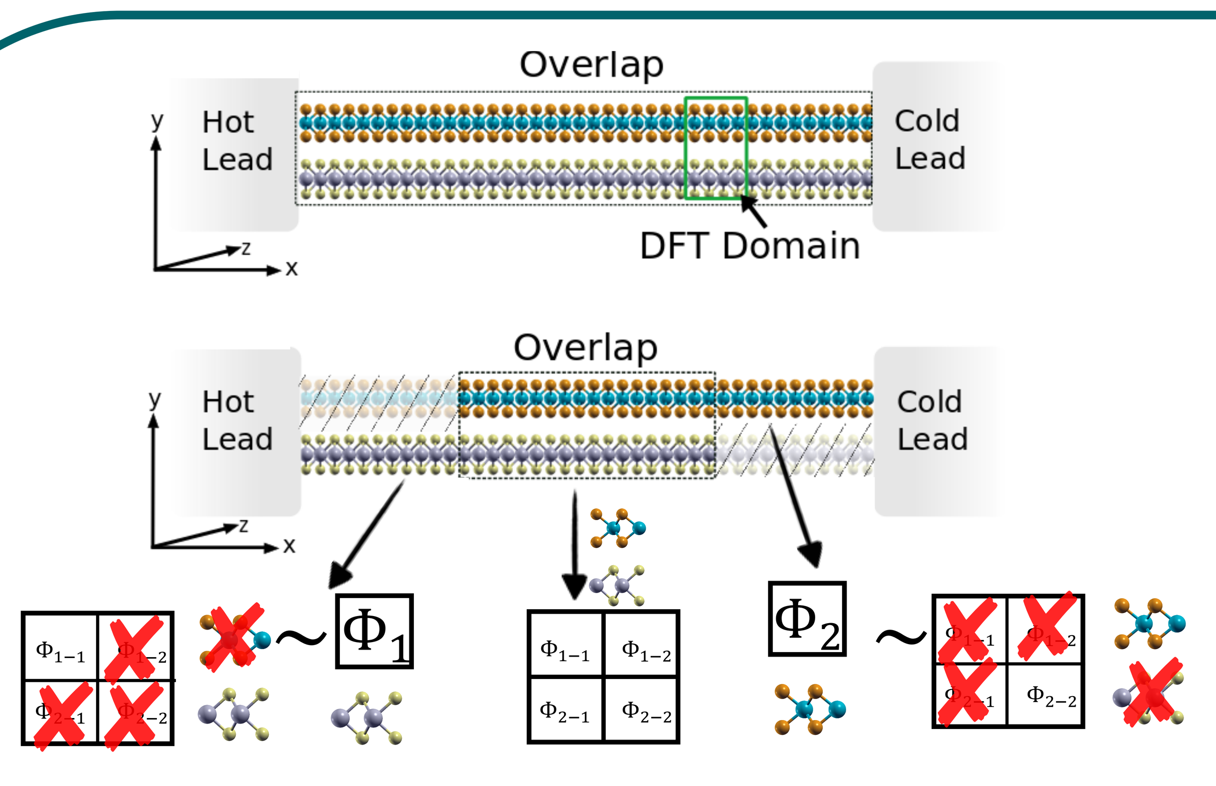
Homo-bilayers	Hetero-bilayers
TMD_1=TMD_2	$TMD_1 \neq TMD_2$
MoS_2-MoS_2	MoS_2-$MoSe_2$
$MoSe_2$-$MoSe_2$	MoS_2-WS_2
$MoTe_2$-$MoTe_2$	MoS_2-WSe_2
WS_2-WS_2	$MoSe_2$-WS_2
WSe_2-WSe_2	MoS_2-WSe_2
	WS_2-WSe_2

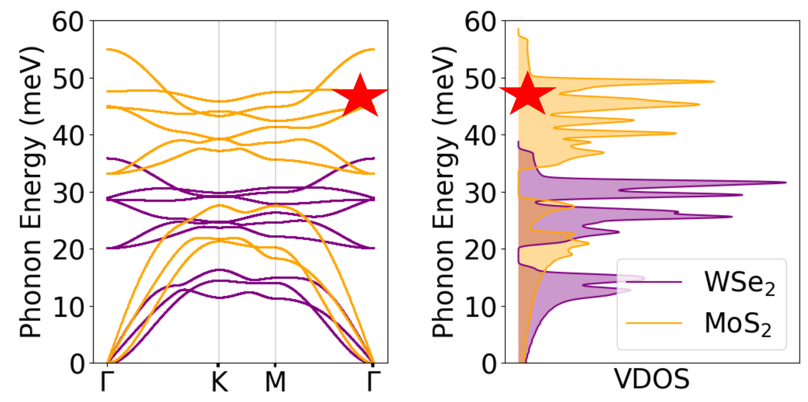
Device Configurations



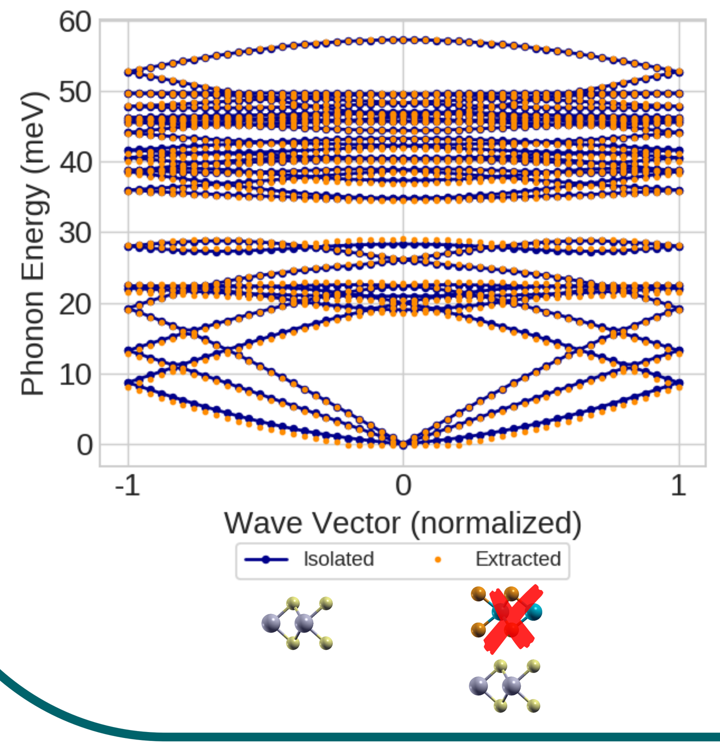
Previous electronic characterizations (theoretical [2] and experiments [3-4]) showed that such setups favour inter-layer band-to-band tunnelling and can therefore be used as field-effect transistors with a potentially *steep subthreshold swing* and a *high ON-state current*.

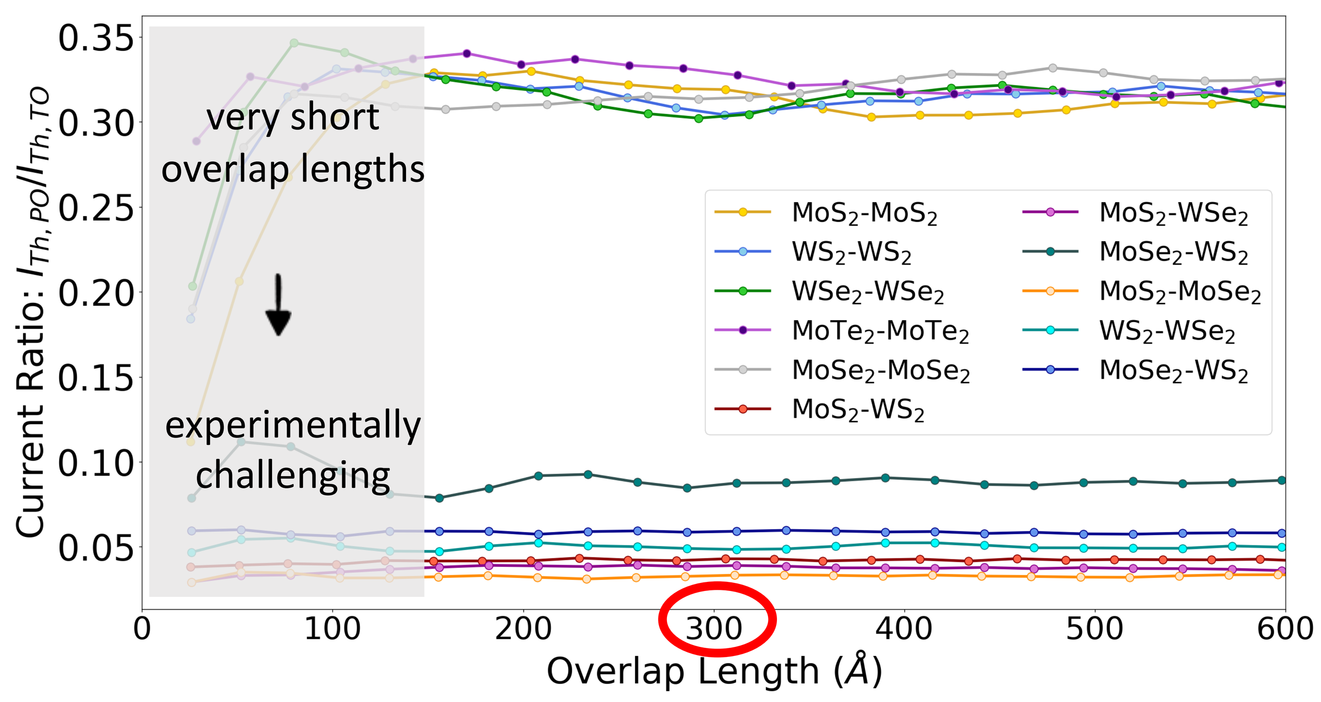
Simulation Results and Analysis





In the ballistic limit of transport only states existing throughout the whole structure can be transmitted from one contact to the other [5]





- The properties of each individual layer can be retrieved from those of the stack
- $|I_{Th,TO} - (I_{Th,1} + I_{Th,2})| < 10\%$ (TO, 1+2)
- Structures with a partial overlap can be created by starting from a TO vdWM from which the atoms/Φ entries corresponding to the extra layer can be removed
- Results are independent of the overlap length
- Dominant contribution of acoustic phonons
- Structures with a partial overlap act as a filter

Homo-bilayers	Hetero-bilayers
$I^{(n)}_{Th,PO}(\hbar\omega) \sim 0.3 I^{(n)}_{Th,TO}(\hbar\omega)$	$I^{(m)}_{Th,PO}(\hbar\omega) \sim 0.05 I^{(m)}_{Th,TO}(\hbar\omega)$
$I^{(n)}_{Th,PO}(\hbar\omega) \sim 0.6 I^{(n)}_{Th,1(2)}(\hbar\omega)$	$I^{(n)}_{Th,PO}(\hbar\omega) \ll I^{(n)}_{Th,1(2)}(\hbar\omega)$
$\mathcal{T}^{(n)}_{PO}(\hbar\omega) \sim 0.3 \mathcal{T}^{(n)}_{TO}(\hbar\omega)$	$\mathcal{T}^{(m)}_{PO}(\hbar\omega) \sim \mathcal{T}^{(m)}_{TO}(\hbar\omega)\mathcal{F}(\hbar\omega)$

Conclusions

Our work emphasizes the possibility of engineering heat flows at the nanoscale by combining TMD monolayers. It also lays the foundation for future in-depth analysis involving more realistic effects such as anharmonic phonon interactions

CONTACT PERSON

Sara Fiore

Integrated Systems Laboratory, ETH Zurich, 8092 Zurich, Switzerland

safiore@iis.ee.ethz.ch

REFERENCES

[1] Fiore, Sara, and Mathieu Luisier. "Ab initio modeling of thermal transport through van der Waals materials." *Physical Review Materials* 4.9 (2020): 094005. https://link.aps.org/doi/10.1103/PhysRevMaterials.4.094005
[2] A. Szabo, S. J. Koester, and M. Luisier, "Ab-initio sim-ulation of van der Waals MoTe2–SnS2 heterotunnelingFETs for low-power electronics,"IEEE Electron DeviceLetters, vol. 36, no. 5, pp. 514–516, 20
[3] X. Yan, C. Liu, C. Li, W. Bao, S. Ding, D. W. Zhang, andP. Zhou, "Tunable snse2/wse2 heterostructure tunnelingfield effect transistor,"Small, vol. 13, no. 34, p. 1701478,2017.
[4] T. Roy, M. Tosun, X. Cao, H. Fang, D. Lien, P. Zhao,Y. Chen, Y. Chueh, J. Guo, and A. Javey, "Acs nano2015, 9, 2071–2079
[5] E. Gnani, A. Gnudi, S. Reggiani, M. Luisier, and G. Bac-carani, "Band effects on the transport characteristics ofultrascaled snw-fets,"IEEE Transactions on Nanotechnology, vol. 7, no. 6, pp. 700–709, 2008.

Graphene online 2020