Transmission Fast Atom Diffraction through 2D materials

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Introduction

- First observation of hydrogen atom diffraction through monocrystalline graphene
- Enables atomic-scale structural analysis of 2D materials using neutral matter waves
- Surface potential mapping

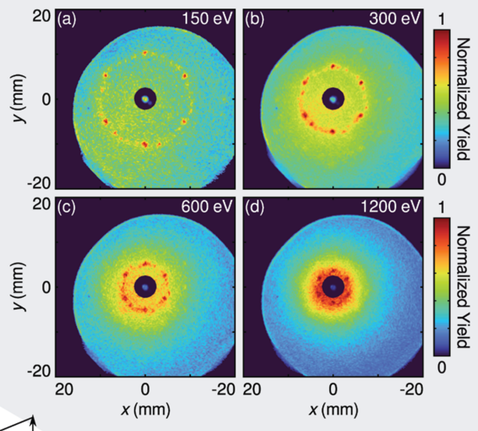
- Eikonal approximation to calculate diffration intensities

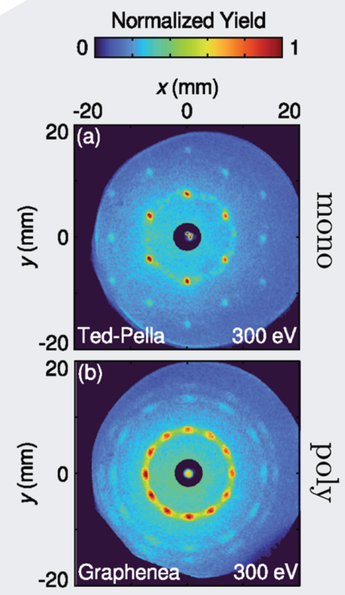
$$I_{m,n} = \left| \frac{1}{\text{Area}} \iint_{\Omega_x,\Omega_y} \mathrm{d}x\mathrm{d}y\, e^{-iG_x x - iG_y y} \exp\left(-\frac{i}{\hbar v_z}\int \mathrm{d}z\, V(x,y,z)\right)\right|^2$$

- Relies on accuracy and computability of the interaction potential

Experimental Results H - Graphene

- Diffraction images for H atoms on single layer graphene
- Clear hexagonal diffraction patterns

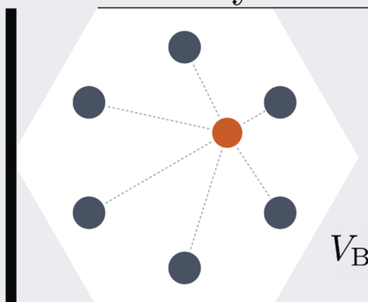




- Multiple domains detection

Theoretical modeling

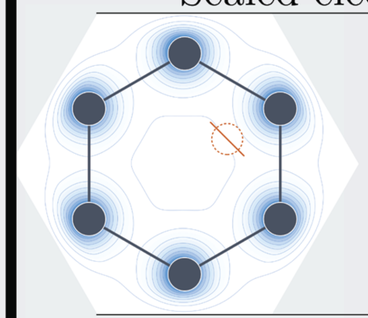
Binary interaction potential



Neglecting interaction between atoms in the surface

$$V_{\text{Binary}} = \sum V_{\text{Probe-Atom}}$$

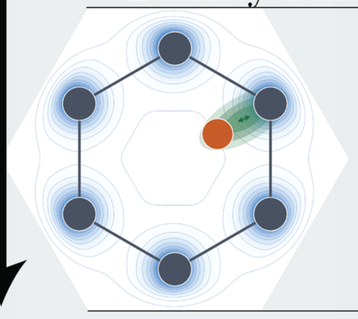
Scaled electron density



Neglecting incoming atom interacting with the surface

$$V_{\text{Scaled}} = \alpha\rho_0$$

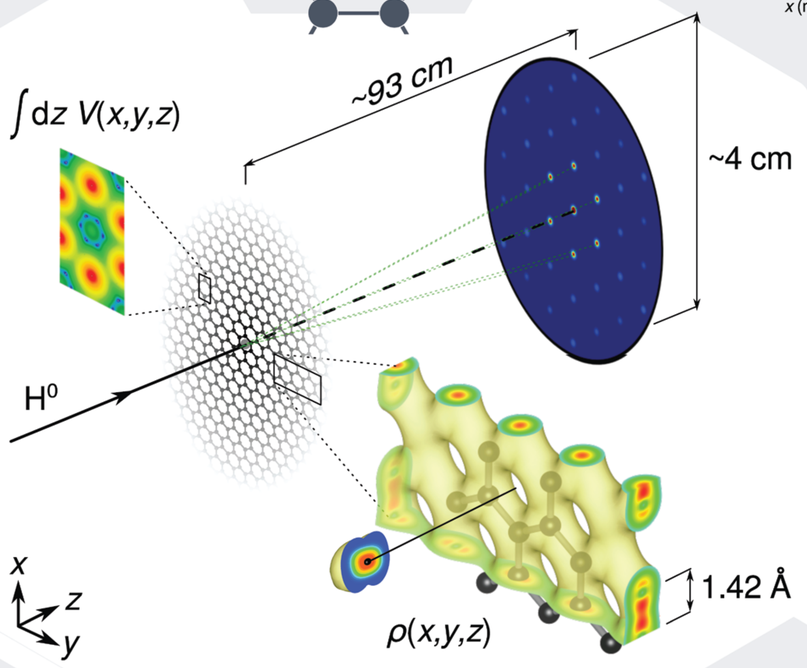
Density Functional Theory

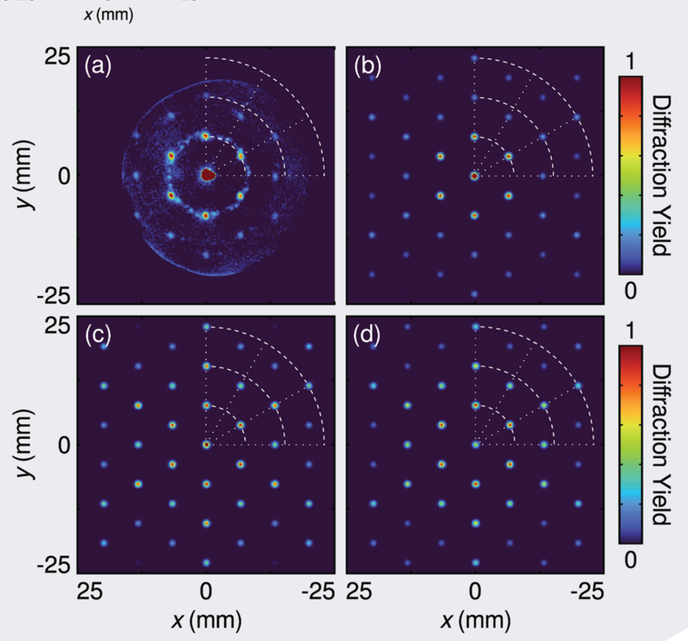


Neglecting the dynamics of the process

$$V_{\text{DFT}} = E_{\text{tot}}[\rho]$$

Enhanced accuracy — Computational cost

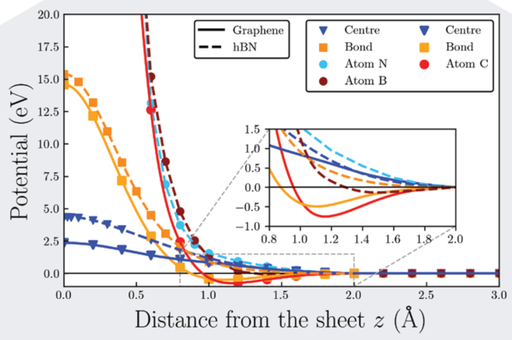




- Only DFT accuracy captures the correct physics

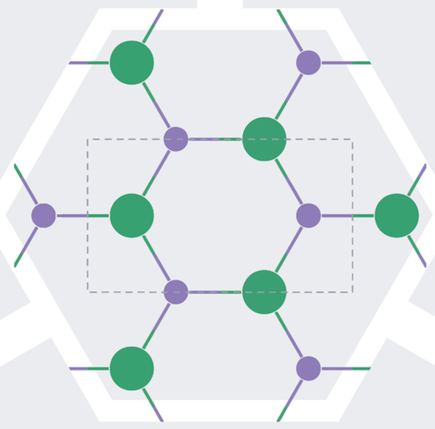
Future development

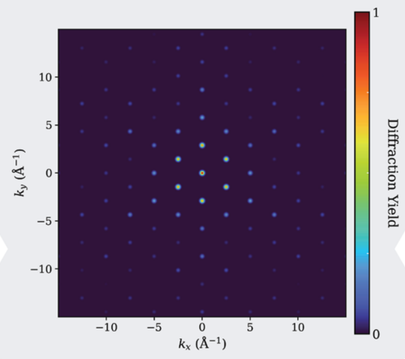
Time-dependent Density Functionnal Theory (TDDFT)

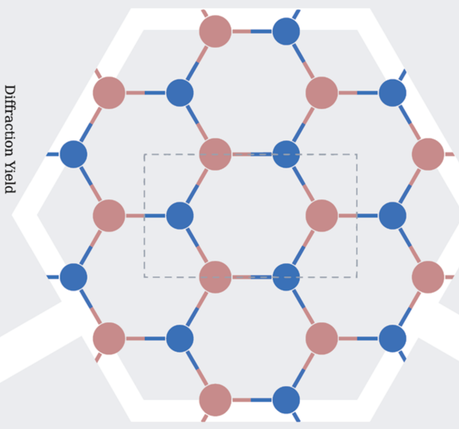


- Can't resolve the two sub-lattices
- Very similar to graphene pattern

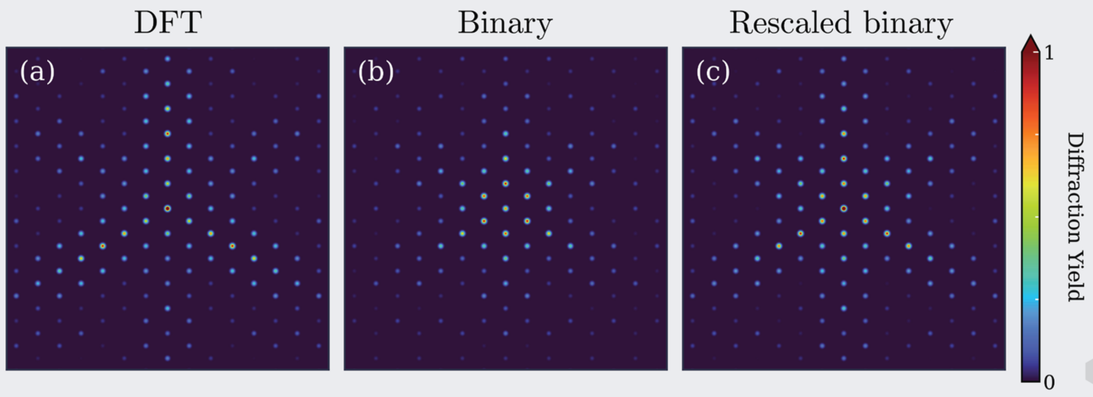
H - hBN





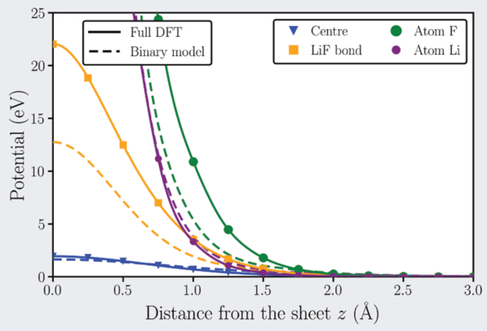


- Highly ordered and rigid ionic lattice



- Charge localisation has an impact on the accuracy of the binary model

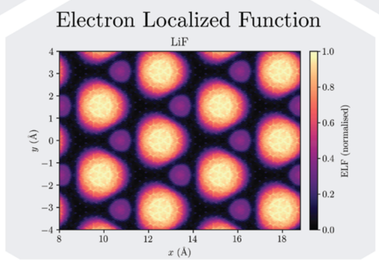
He - LiF



- Two sub-lattices resolved
- Scaling binary interaction works for Alkali Halides

Take home message

- Transmission of fast hydrogen atoms through graphene is only correctly modeled by DFT level interaction potential
- Other surfaces and incoming atoms can be studied
- This is an **interaction spectroscopy**



References

[1] C. Kanitz, *et al*, Diffraction of helium and hydrogen atoms through single-layer graphene. Science 2025
[2] P. Guichard, *et al*, Fast Hydrogen Atom Diffraction through Monocrystalline Graphene. Physical Review Letters 2025