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Nanoscale Optoelectronic Materials through Theoretical Modeling

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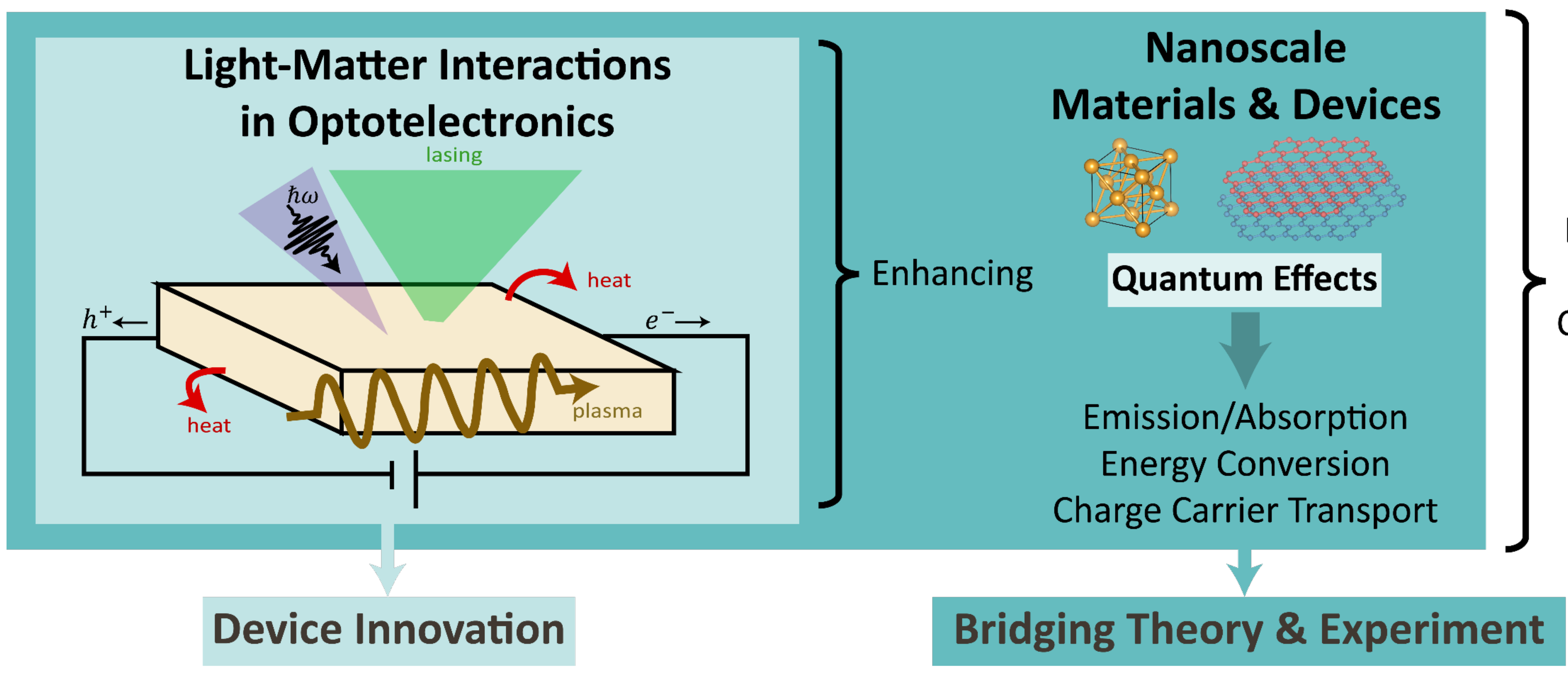
Background and Motivation



First Principle Atomic Scale Density Functional Theory Calculation

Electrical properties

Electrical contacting **unbalance** and limitations to control **contacting properties**:

- **4H-SiC with ALD ZnO**

Optical properties

Low-dimensional materials considering **weak interaction** (Van der Waals force):

- **mono- and twisted bi-layer graphene**

Rationale of Optoelectronic Devices Innovation

Work function Tunning of 4H-SiC by Atomic-level ZnO interlayer

Hexagonal polytypes of SiC (4H-SiC, 6H-SiC):

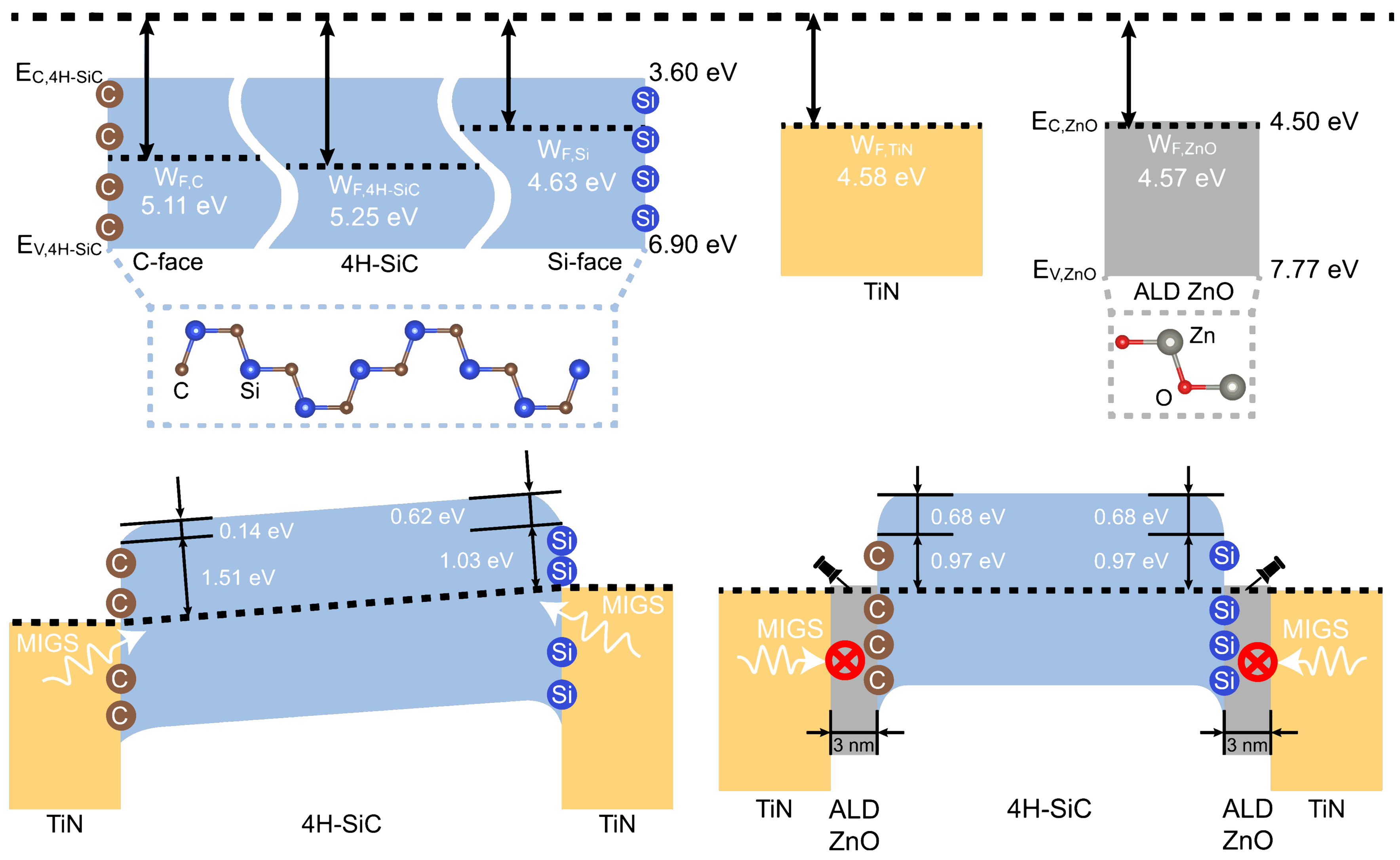
- **Polarity** at atomic layer-by-layer growth surfaces (0001) and $(000\bar{1})$
- **Dangling unsaturated** sp^3 hybridization bonds

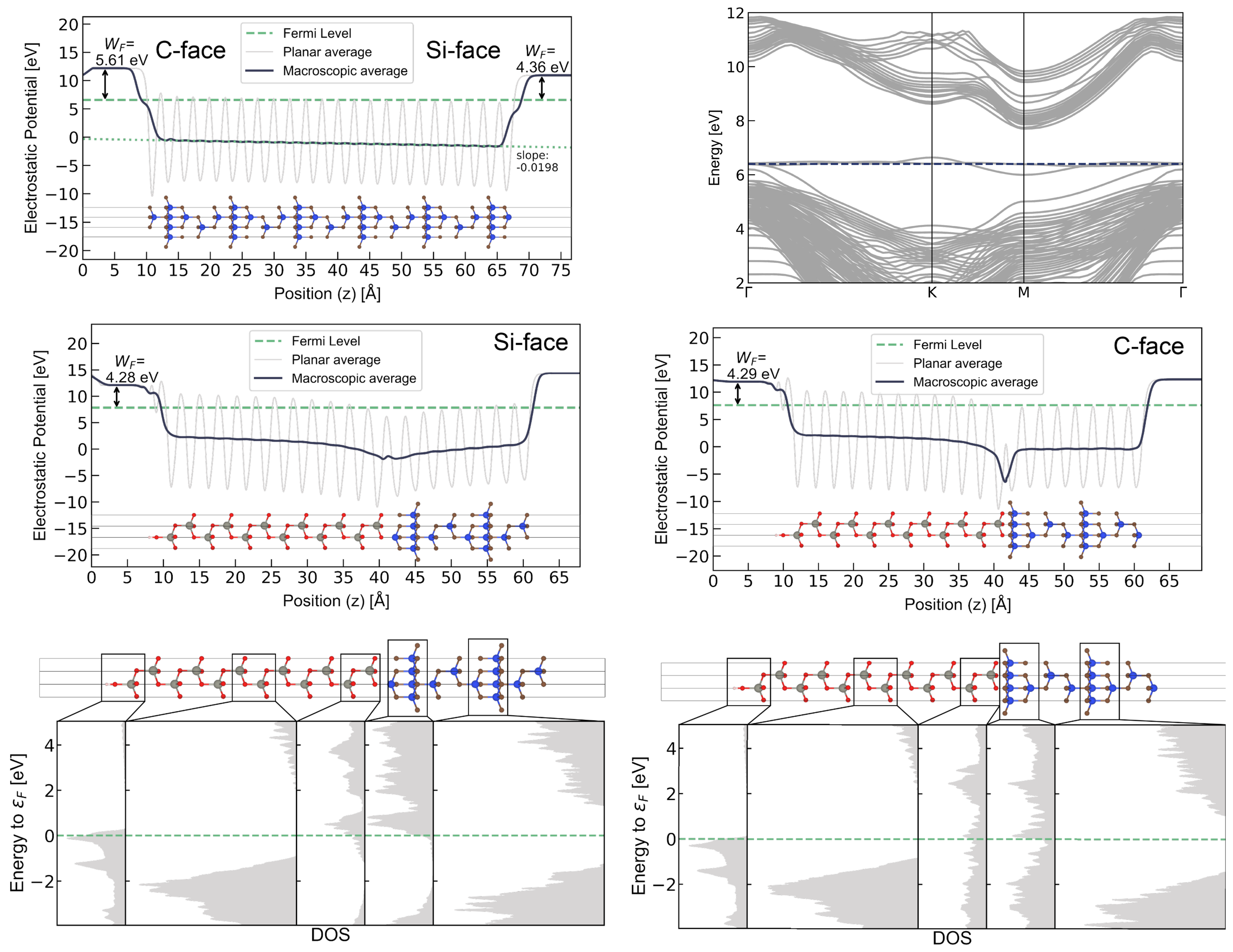
Resulting in

- **Spontaneous polarization**
- **Imbalanced surface potential**
- **Strong surface states**

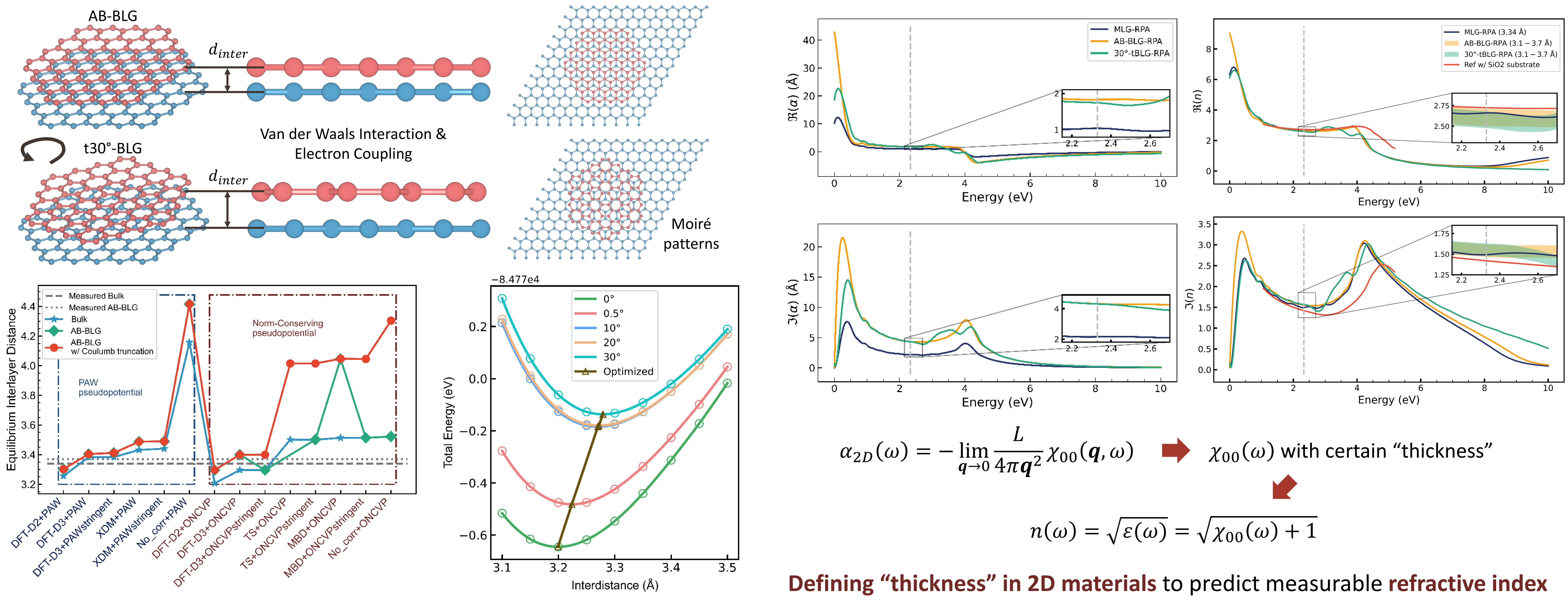
ALD ZnO can solve

Berry Phase Calculation (Polarization)	4H-SiC (z-axis 10.11 Å)	ZnO (z-axis 5.20 Å)
	$1.8965\ C/m^2$ per unit cell	$0.9176\ C/m^2$ per unit cell





Optical Response of Twisted Bilayer Graphene



$$\alpha_{2D}(\omega) = -\lim_{q\to 0}\frac{L}{4\pi q^2}\chi_{00}(q,\omega) \Rightarrow \chi_{00}(\omega) \text{ with certain "thickness"}$$

$$n(\omega) = \sqrt{\varepsilon(\omega)} = \sqrt{\chi_{00}(\omega)+1}$$

Defining "thickness" in 2D materials to predict measurable **refractive index**

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