Midgap state in SiC monolayer induced by atom adsorption

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1 Introduction

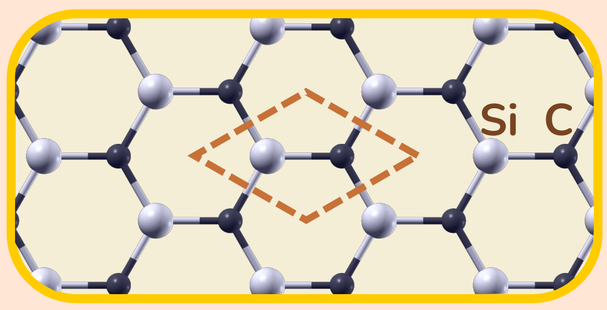
A recent synthesis of two-dimensional silicon carbide (2D-SiC) expanded the family of 2D honeycomb materials with a new 2D semiconductor. By performing density functional calculations, we demonstrate that the Si atom displacement modifies the electronic structure of 2D-SiC and induces the midgap state that can accommodate two electrons with opposite spins. We show that the adsorption of Li and Ca atoms creates the local deformation at the adsorption site and induces the midgap electronic state. This interplay of structural distortion and electronic properties provides a strategy to tailor the bandgap of 2D-SiC, candidating it for applications in ultrathin field-effect transistors.

2 Silicon carbide monolayer

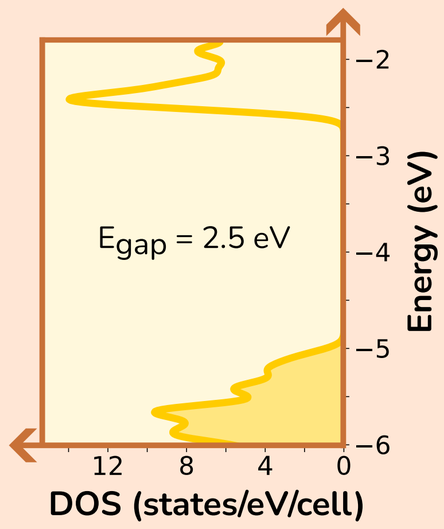
Methodology:

- Density functional theory (DFT) calculations with GPAW
- Supercell approach with periodic boundary conditions

2D-SiC is a monolayer (ML) crystal structure with a honeycomb lattice.



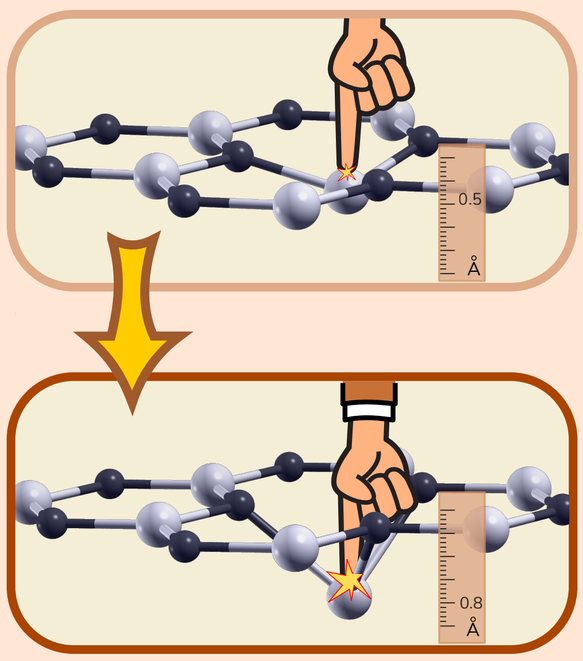
SiC crystal lattice with dashed unit cell



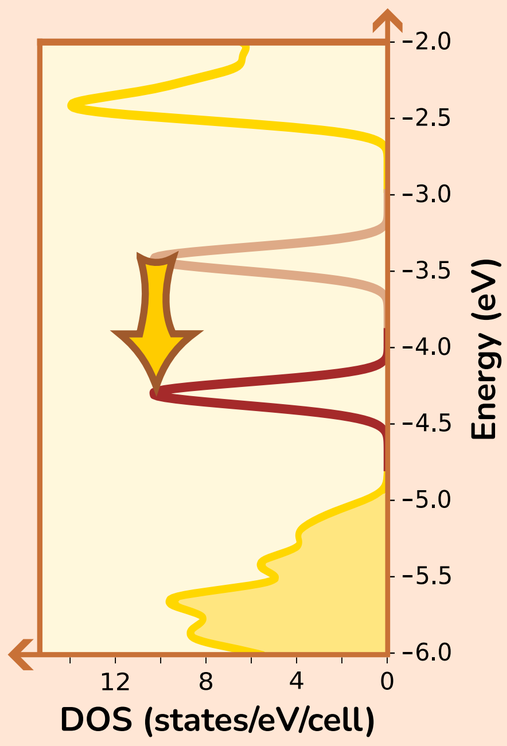
Total DOS of SiC ML

3 Midgap state

Out of plane displacement of a single Si atom creates a localized midgap state that can accommodate two electrons with opposite spins.



Gradual deformation of SiC

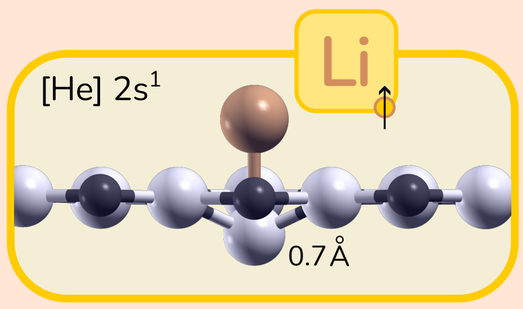


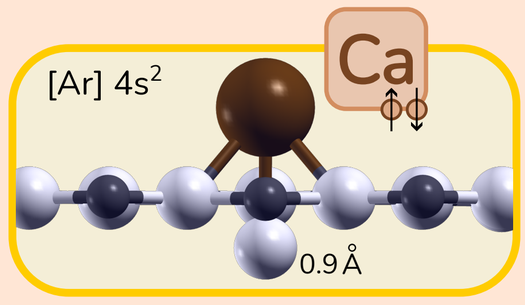
Total DOS of pristine (yelow) and deformed SiC (brown)

Increasing the displacement of the silicon atom shifts a midgap state from the bottom of the conduction band towards the valence band.

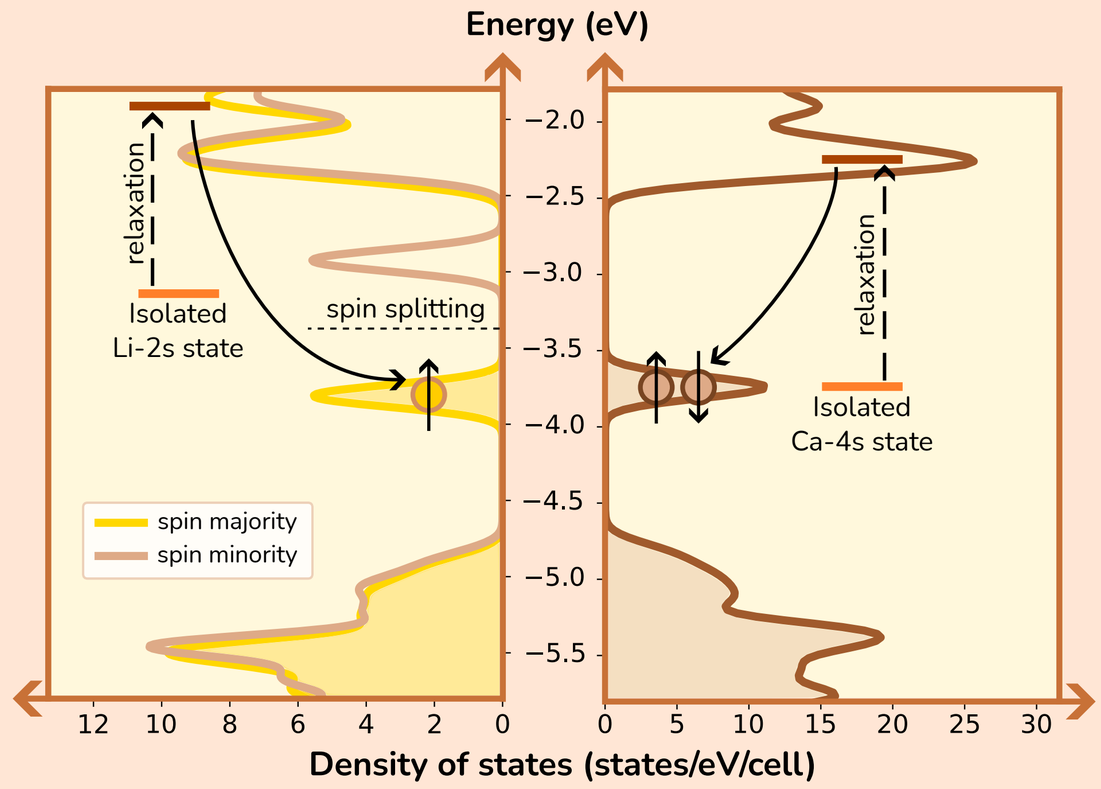
4 Adsorption of Li and Ca atoms

The midgap state can be experimentally realized by the adsorption of atoms with low electronegativity, that can easily donate electrons to SiC. Since the state can be filled with one or two electrons our choice are lithium and calcium atoms.





Both Li and Ca atoms bind on top of the Si atom creating a local deformation. Electron transfer from the atomic (Li-2s, Ca-4s) to the lower midgap state stabilizes the system and overcomes the energy cost of deformation.



Spin resolved total DOS of Li on SiC (left) and total DOS of Ca on SiC (right)

5 Conclusion

- ✓ Out of plane dispacement of Si atom creates a midgap state.
- ✓ Increasing displacement of Si atom shifts the midgap state downwards on the energy scale.
- ✓ Li fills the midgap state with one and Ca with two electrons.

References

1. S. Chabi, et al., Nanomaterials **11**, 1799 (2021).
2. M. Orozović, Ž. Šljivančanin and S. Stavrić, manuscript in preparation.
3. S. Stavrić, Z. S. Popović and Ž. Šlijvančanin, Phys. Rev. Mater. **2**, 114007 (2008).

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