Small organic molecule adsorbed silicene

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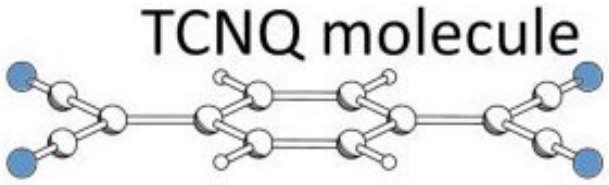
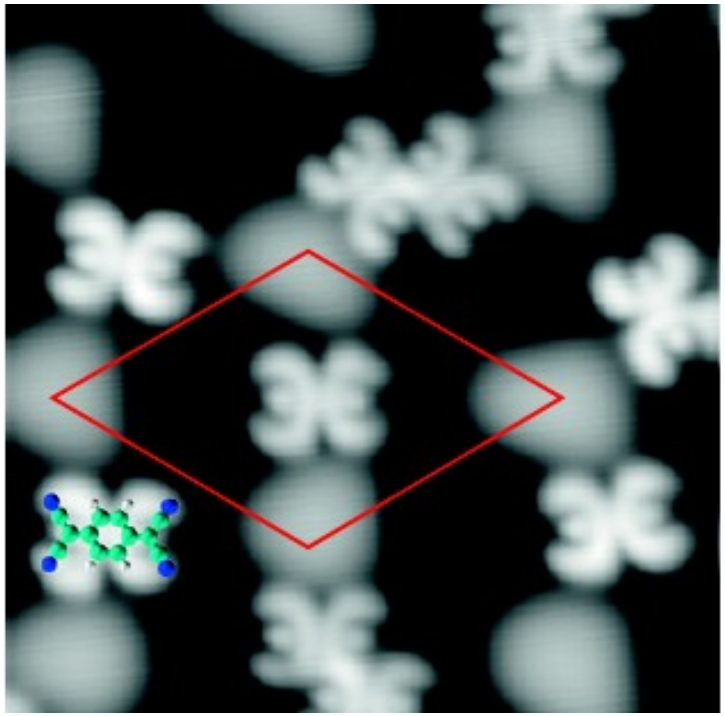
Motivation



Tetracyano-quinodimethane



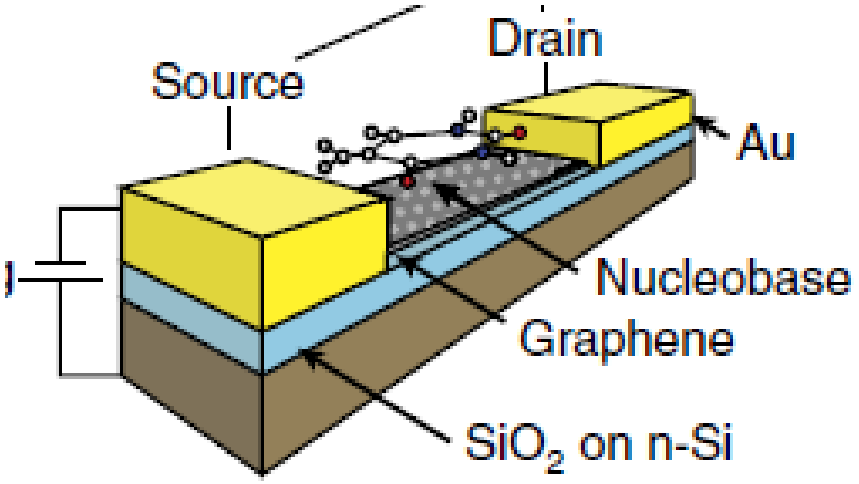
Nat. Phys. 9, 368 (2013)

Vol 454|17 July 2008|doi:10.1038/nature07094 nature

LETTERS

Imaging and dynamics of light atoms and molecules on graphene

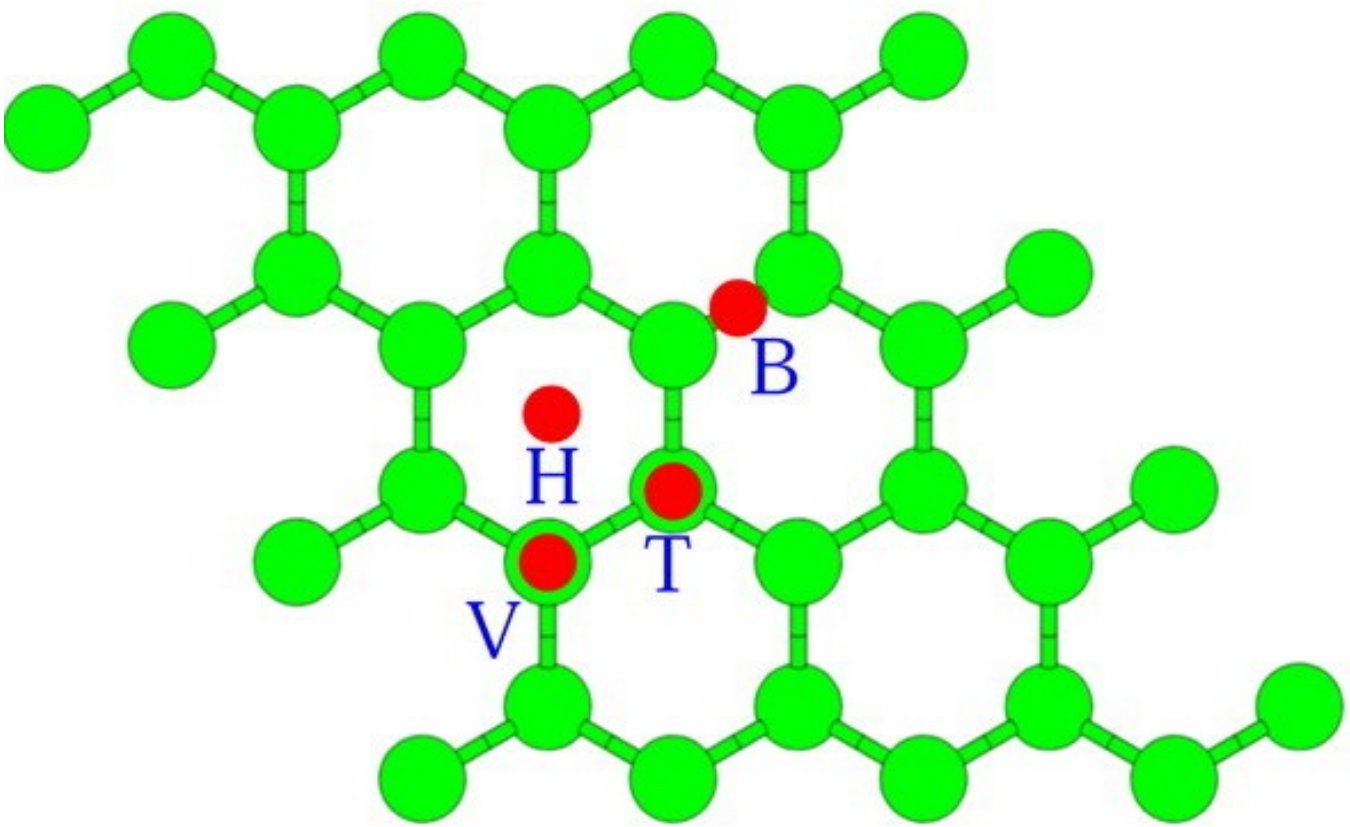
Jannik C. Meyer[1,2], C. O. Girit[1,2], M. F. Crommie[1,2] & A. Zettl[1,2]



Nat. Commun. 6, 6563 (2015)

Weak interaction and problem with the controlling?

Selection criterion for adsorption sites



T. P. Kaloni, J. Phys. Chem. C 118, 25200 (2014)

T. P. Kaloni *et al.,* Phys. Rev. B 89, 035409 (2014)

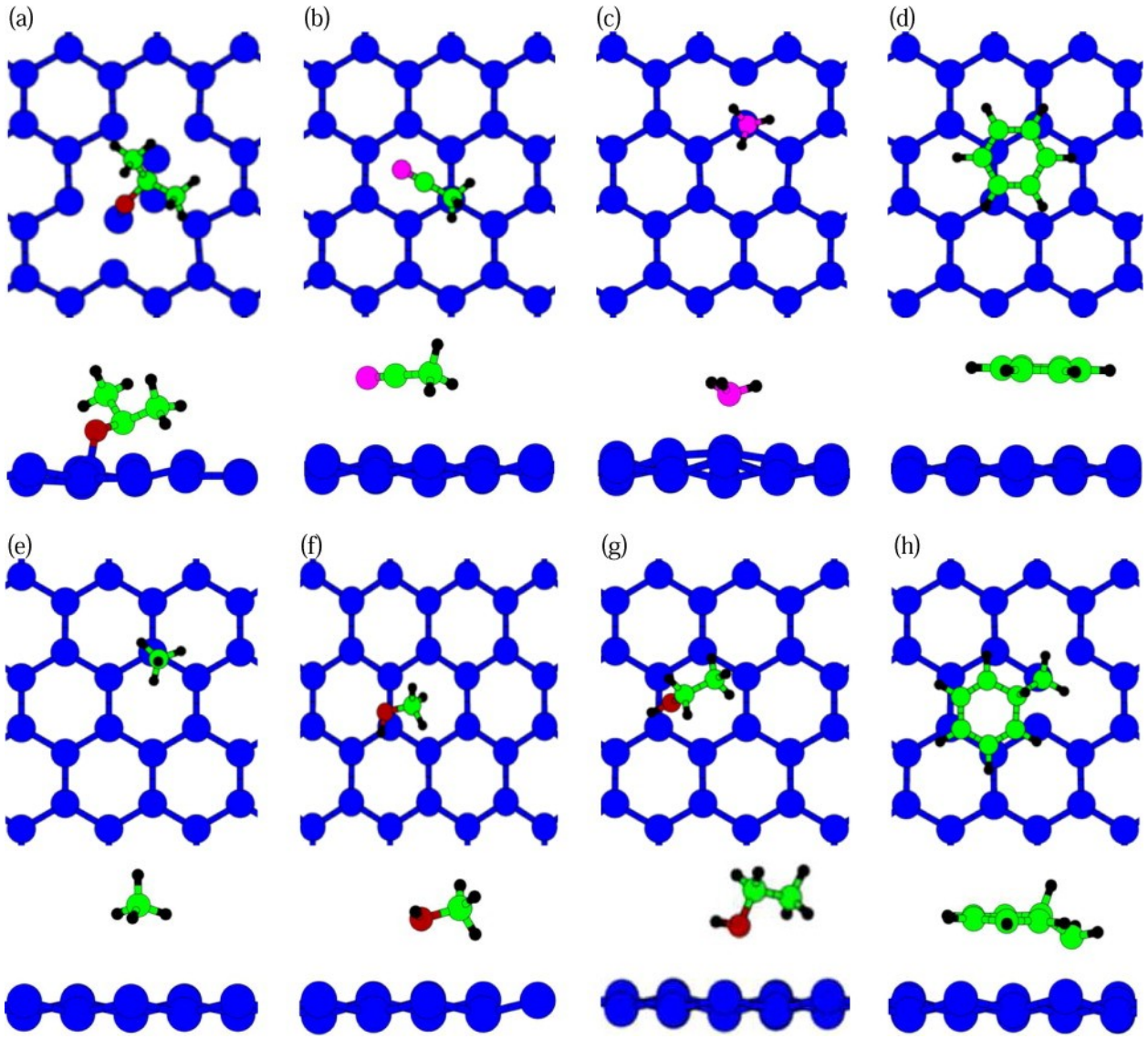
T. P. Kaloni *et al.,* Phys. Rev. B 88, 235418 (2013)

T. P. Kaloni *et al.,* Carbon 64, 281 (2013)

Computational details

- PBE-GGA, implemented in the **Qunatum-ESPRESSO and VASP**
- The van der Waals interaction (DFT-D) is used in order to achieve an accurate description of the dispersion. A high plane wave cutoff energy of 816 eV and a Monkhorst-Pack 24 ×24 × 1 k-mesh
- A 4 ×4 × 1 supercell of silicene with a lattice constant of a = 15.44 Å was employed with a a vacuum layer of 20 Å to avoid artificial interactions due to the periodicity
- The supercell contains 32 Si atoms and a single molecule (acetone, acetonitrile, ammonia, benzene, methane, methanol, ethanol, and toluene) adsorbed on it
- The adsorption density is low enough such that interaction between the molecule and its periodic images is prevented. Atomic positions were optimized until all forces had converged to less than 0.001 eV/Å
- OptB88-vdW functional and the GW approximation have been further used to compare the band gap

Molecular interaction with silicene



Acetone

Acetonitrile

Ammonia

Benzene

Methane

Methanol

Ethanol

Toluene

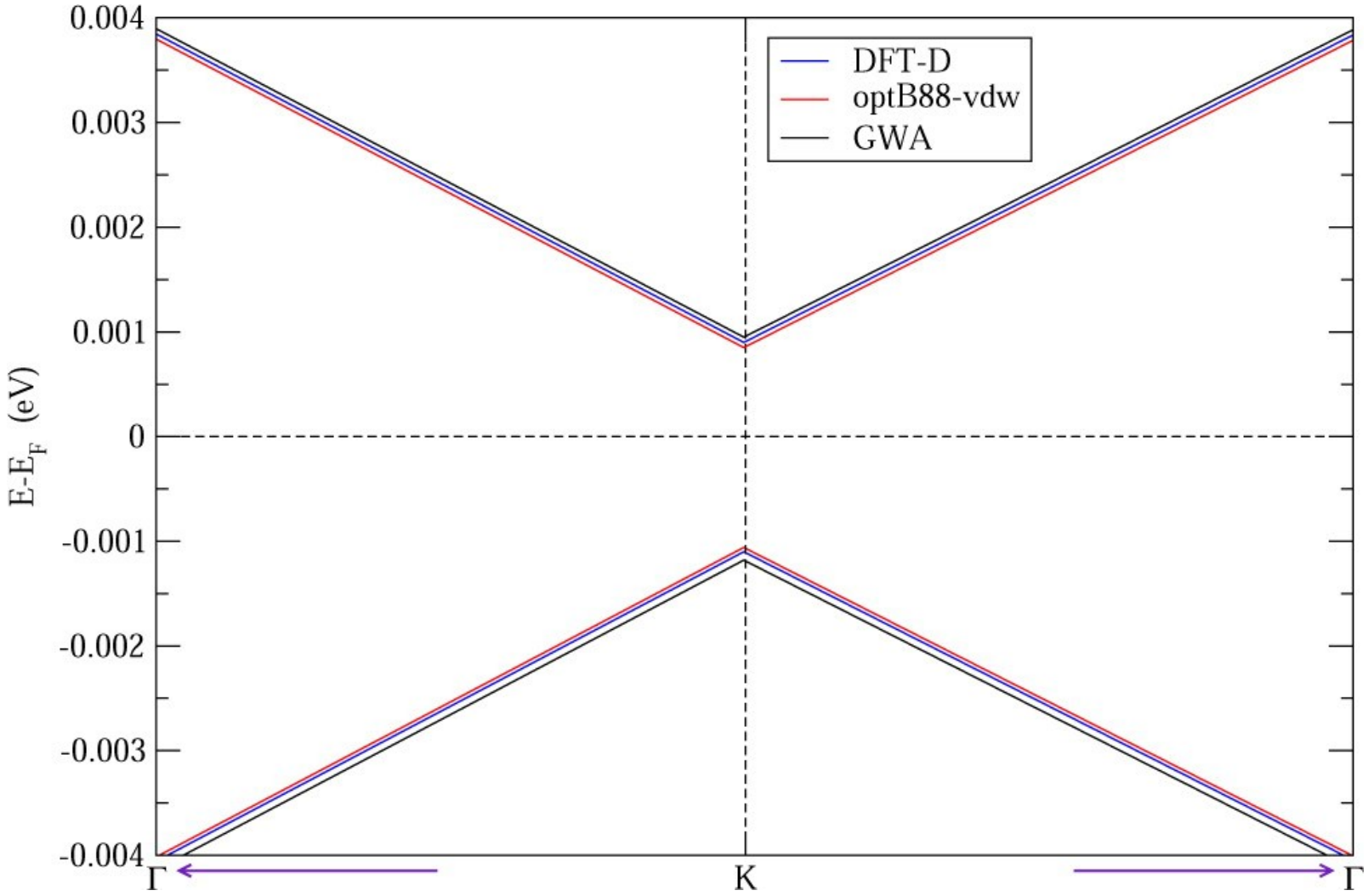
T. P. Kaloni, G. Schreckenbach, and M. S. Freund, J. Phys. Chem. C 118, 23361 (2014)

Structural parameters

system	E_{gap} (eV)	*d* (Å)	θo	Si-Si (Å)	Δ (Å)	m_{eff}
silicene	0.002		116	2.28	0.46	0.001
acetone	0.351	3.04	112-119	2.26-2.36	0.39-0.53	0.166
acetonitrile	0.006	3.38	115-116	2.27-2.28	0.44-0.52	0.003
ammonia	0.103	3.42	113-117	2.27-2.32	0.45-0.51	0.049
benzene	0.007	3.56	114-116	2.27-2.28	0.42-0.50	0.003
methane	0.002	3.10	113-117	2.27-2.28	0.42-0.58	0.001
methanol	0.011	3.48	115-117	2.27-2.28	0.45-0.50	0.005
ethanol	0.017	3.22	114-116	2.27-2.29	0.44-0.49	0.008
toluene	0.208	3.41	113-117	2.26-2.29	0.42-0.48	0.098

T. P. Kaloni, G. Schreckenbach, and M. S. Freund, J. Phys. Chem. C 118, 23361 (2014)

Effect of functionals in the band gap



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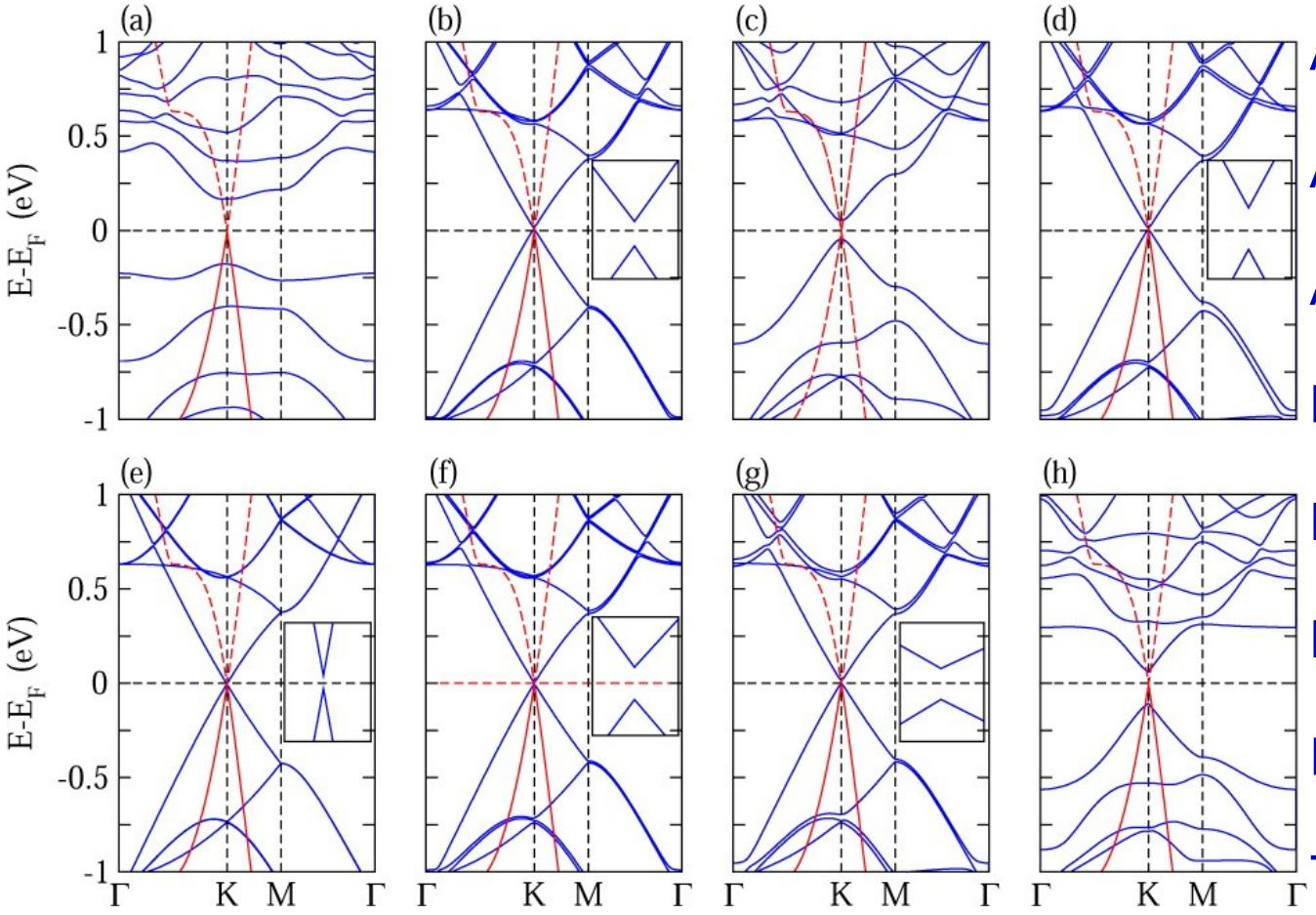
Electronic Structure



Acetone (0.351 eV)

Acetonitrile (0.006 eV)

Ammonia (0.103 eV)

Benzene (0.007 eV)

Methane (0.002 eV)

Methanol (0.011 eV)

Ethanol (0.017 eV)

Toluene (0.208 eV)

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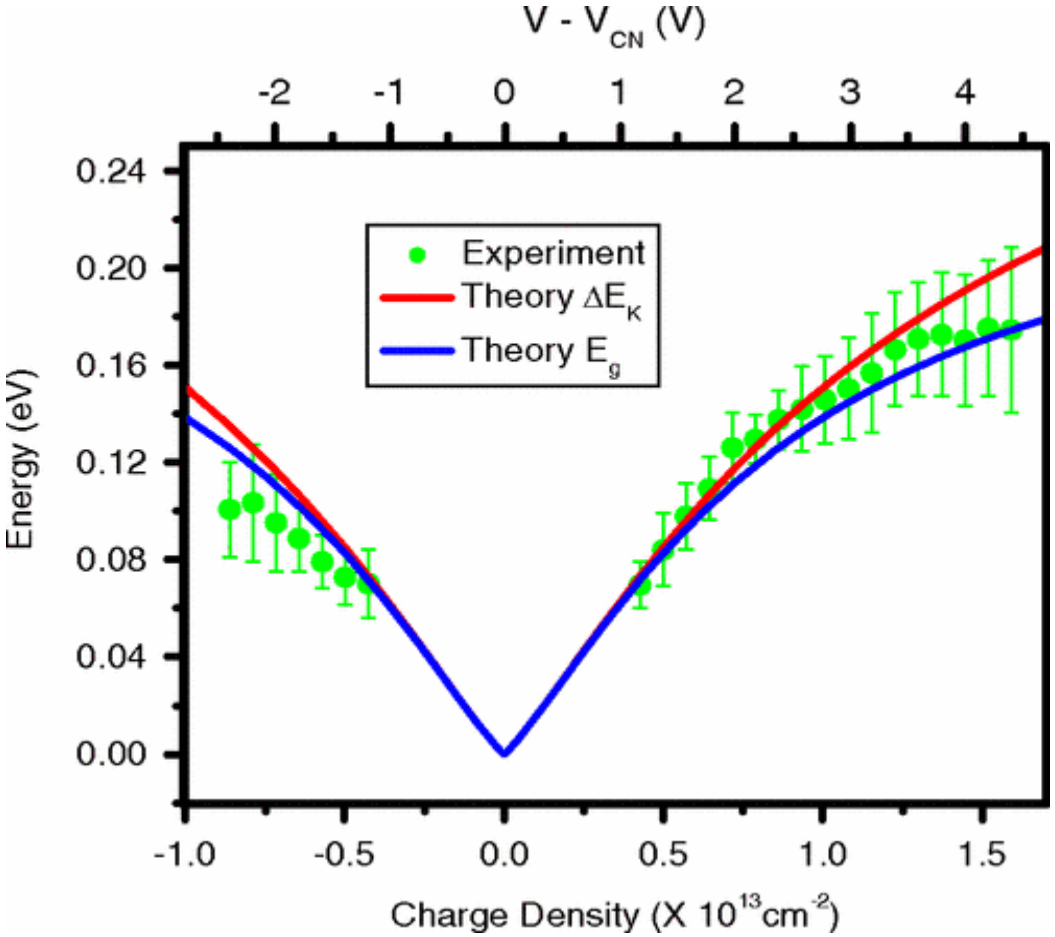
Charge transfer create internal electric field



Phys. Rev. Lett. 102, 256405 (2009)

$$E_{field} = \frac{2Q}{\epsilon_0 a^2 \sin(\pi/3)}$$

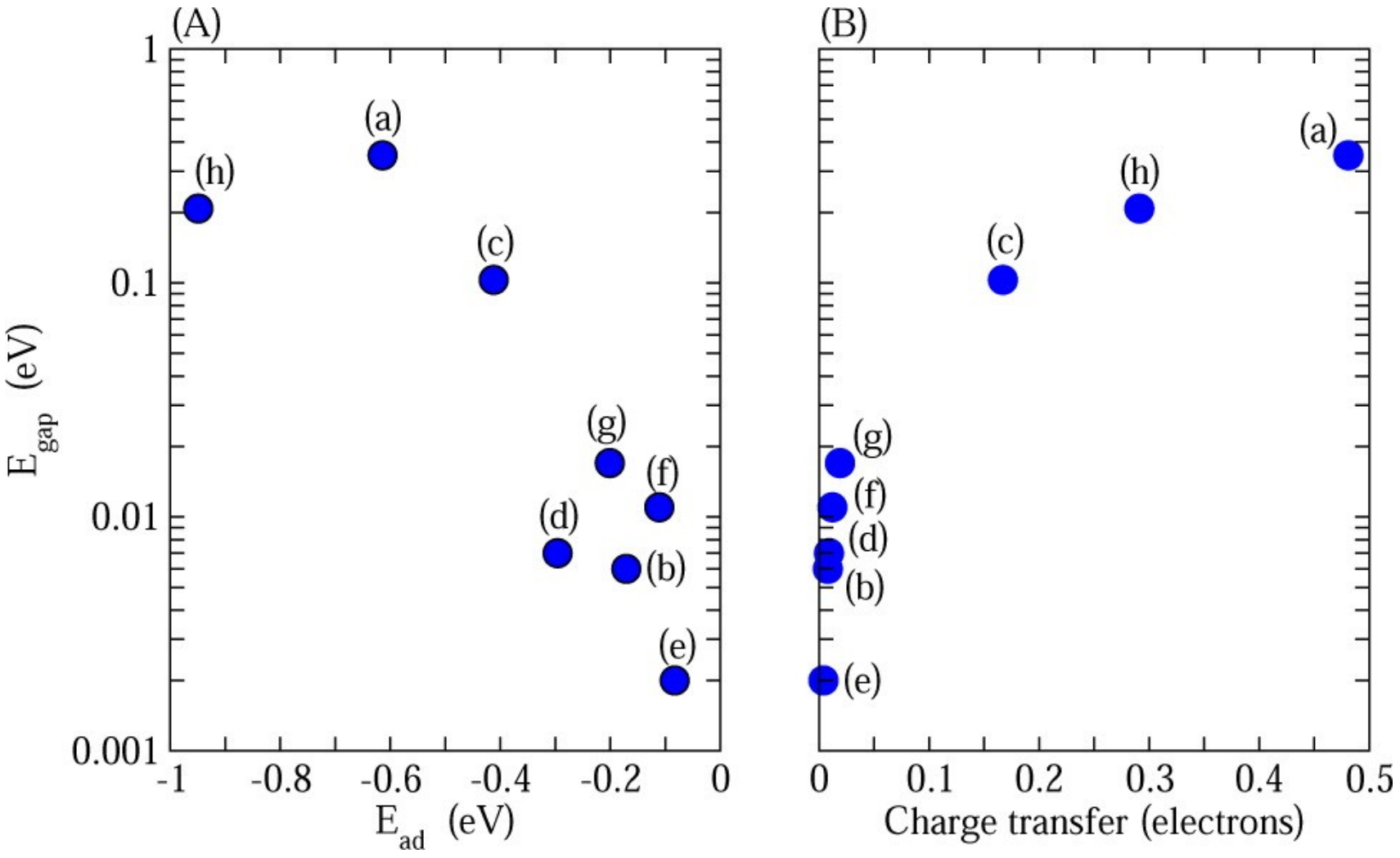
Nano Lett. 12, 113 (2012)

Physica E 59, 60 (2014)

T. P. Kaloni *et al*. Sci. Rep. 3, 3192 (2013)

T. P. Kaloni *et al.* J. Phys. Chem. C 119, 11896 (2015)

Band gap vs. charge transfer



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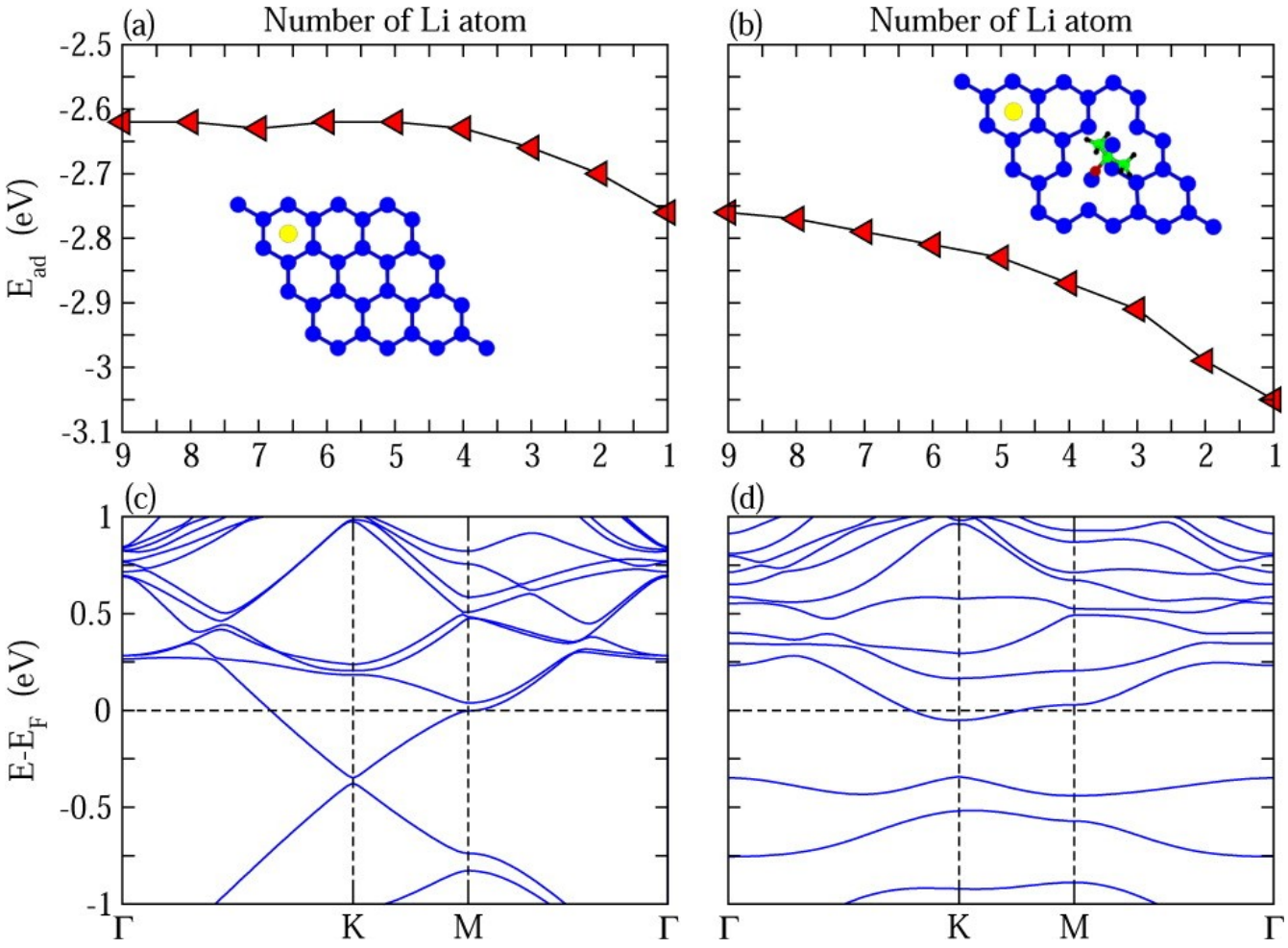
Li in pristine and acetone adsorbed silicene



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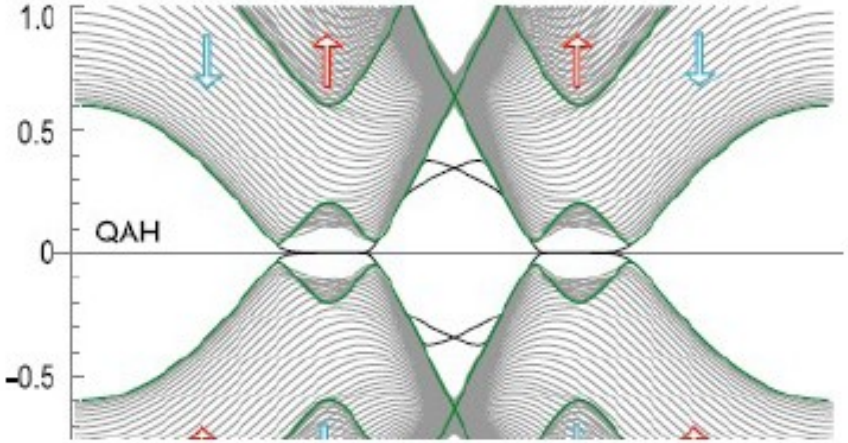
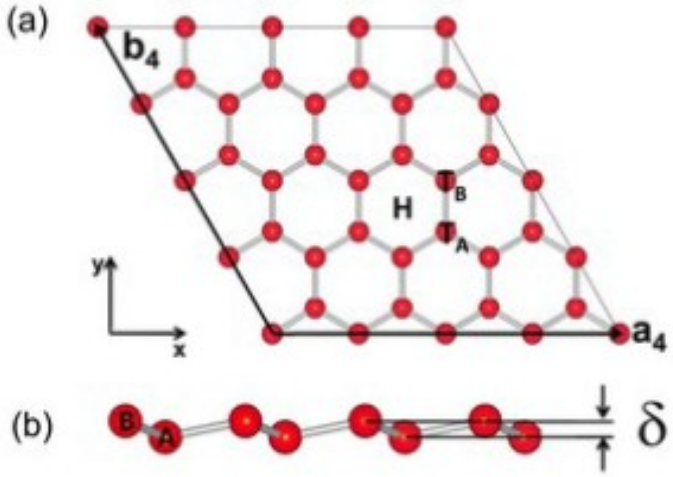
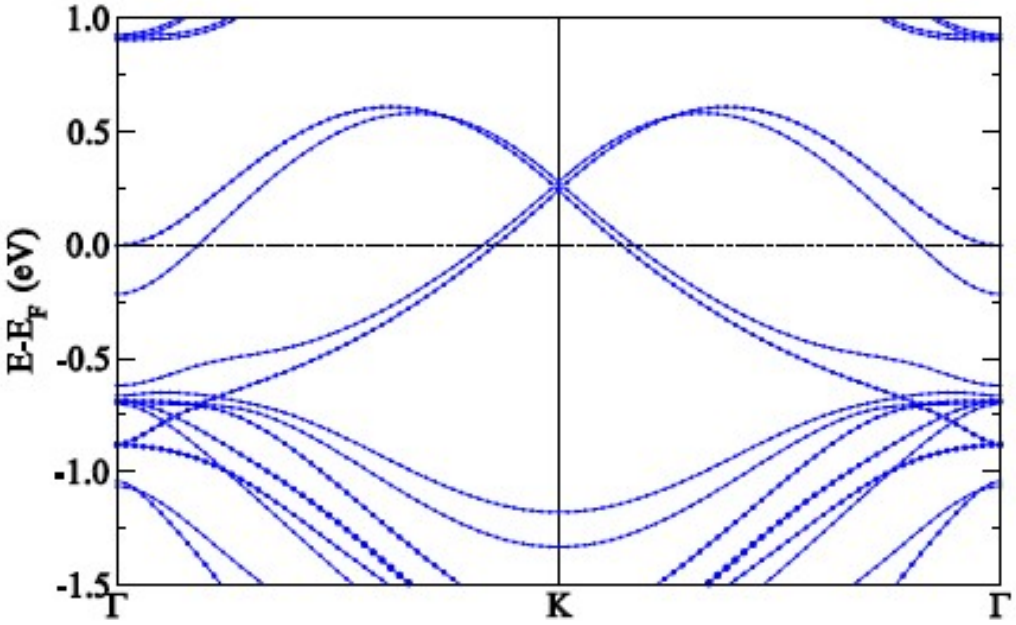
Quantum anomalous Hall (QAH) effect





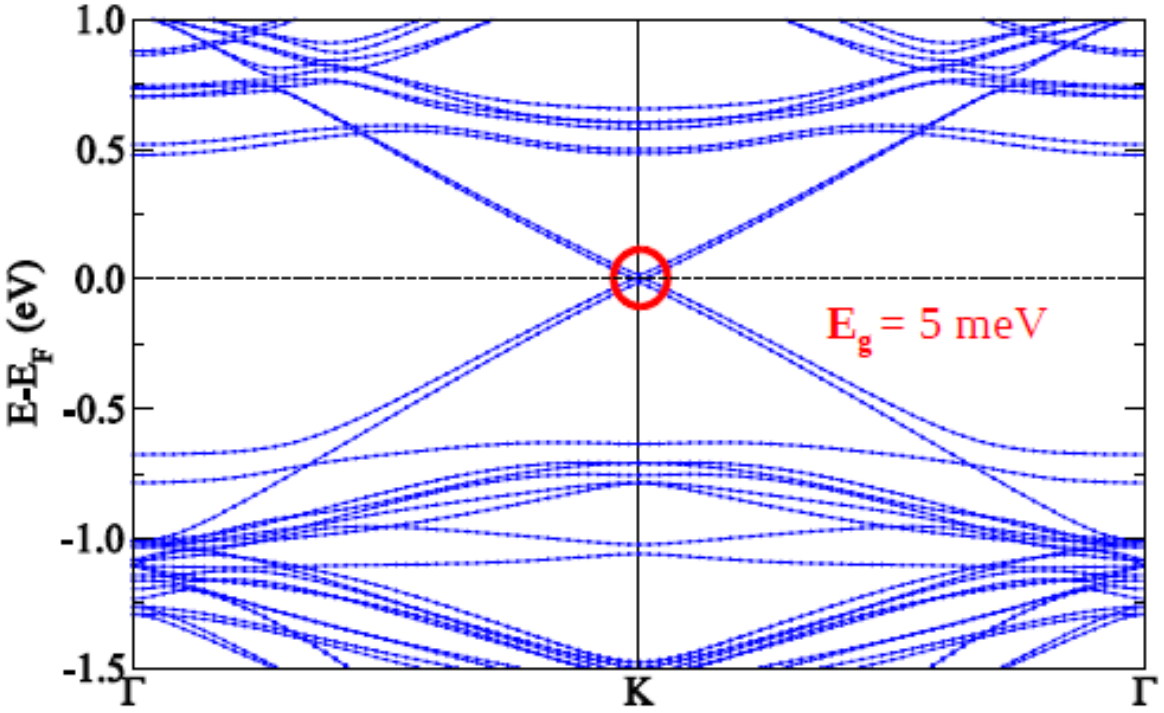


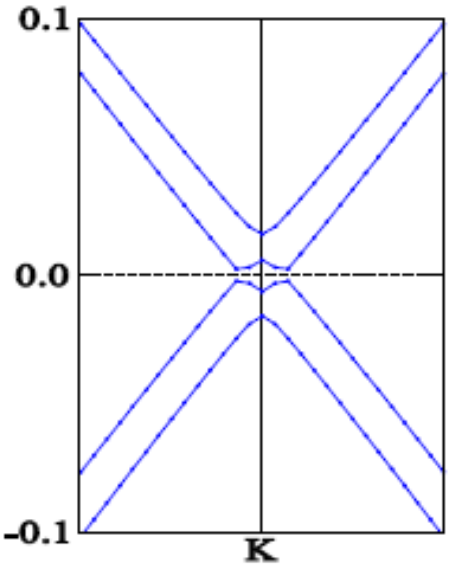
- Ti, V, Cr, Mn, Fe, Co, Ni, Cu, and Zn
- Converge of 75%, 50%,25%, 12.5% and 6.25%
- Hollow site is favourable

Phys. Rev. Lett. **109**, 055502 (2012)

T. P. Kaloni *et al.*, Phys. Rev. B **89**, 035409 (2014)

QAH effect in Co-decorated silicene



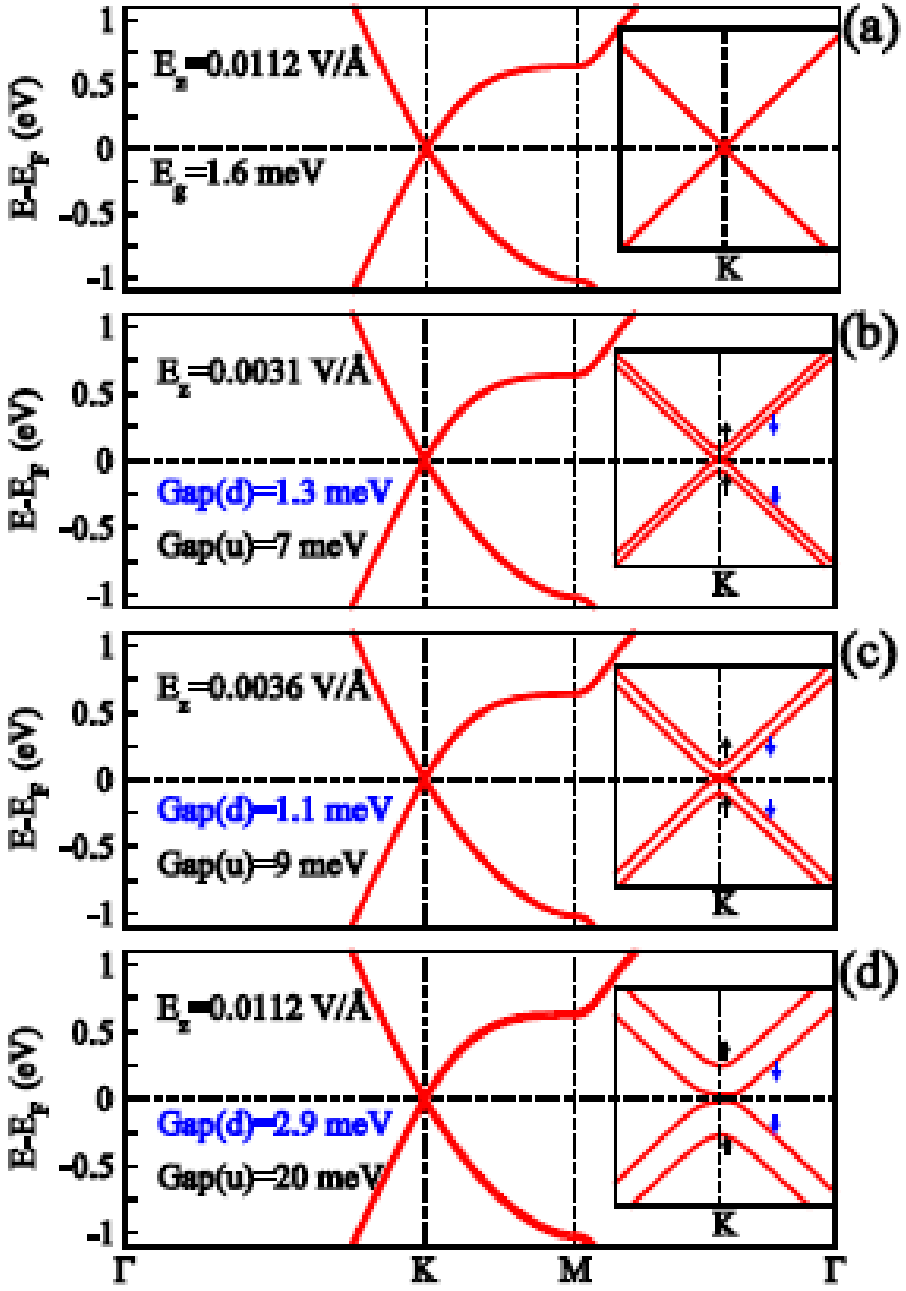


- No hybridization between the 3*d* (TM) and 4*s* (Si)
- No distortion in silicene sheet as compared to other atoms
- Induced SOC and exchange field is suitable

- Internal magnetization breaks the time-reversal symmetry and
- SOC induces the band inversion

T. P. Kaloni *et at*., Phys. Rev. B **89**, 035409 (2014)

Phase transition in silicene



Pristine silicene

Topological insulator
(E_z < SOC)

Semi-metal
(E_z = SOC)

Band insulator
(E_z > SOC)

T. P. Kaloni *et al.*, Sci. Rep. **3**, 3192 (2013)

Conclusion

- Using van der Waals density functional theory, the structural and electronic properties of acetone, acetonitrile, ammonia, benzene, methane, methanol, ethanol, and toluene adsorbed silicene have been studied

- The adsorption energy found to be higher than those for similar molecules adsorbed graphene, which indicates that silicene could be a better candidate to detect the organic molecules

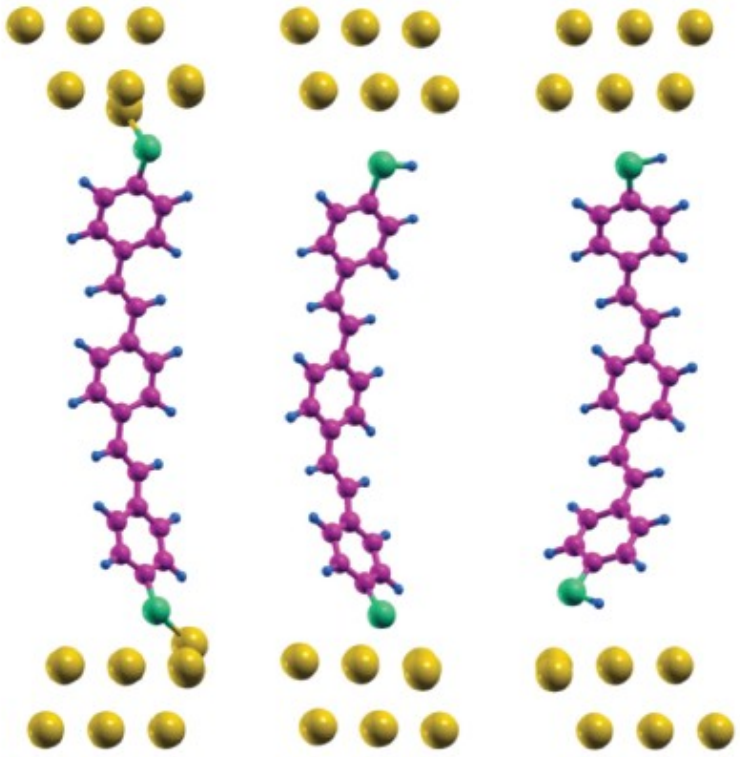
- The calculated band gaps range from 0.006 to 0.35 eV for acetonitrile to acetone. The gap can be increased by applying an electric field, which, could be potential to design the molecular-based electronic devices

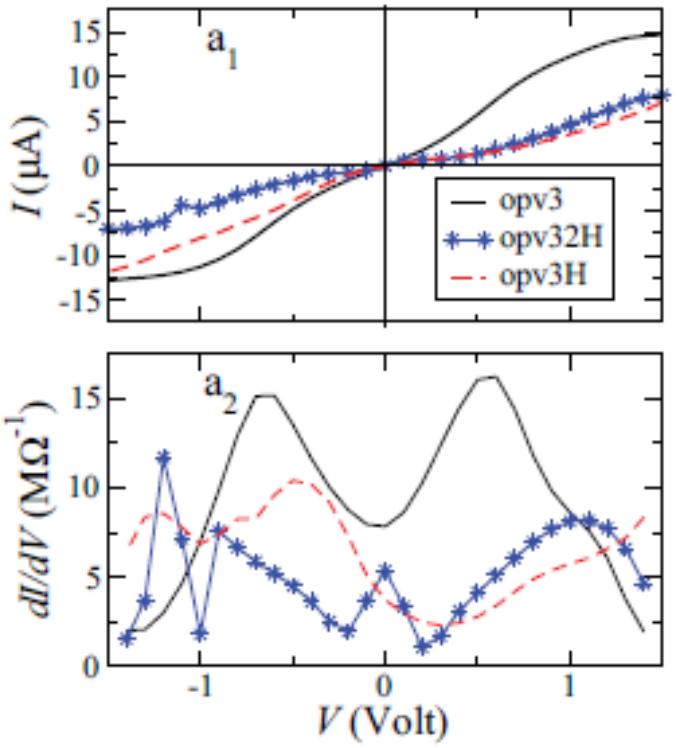
- The effective mass of the electron are found to be smaller as compared to the graphene counterpart, and hence we expect larger mobility, which should be of great importance for silicene-based FETs

- Co-adsorbed silicene can host QAH effect, while phase transition can be obtained by applying an external electric fields in pristine silicene

Future Directions

Transport properties of the materials under study using SIESTA code!





Phys. Rev. B 88, 085438 (2013)

Acknowledgement

- Funding from the Natural Sciences and Engineering Council of Canada (NSERC, Discovery Grant)
- Funding from the Natural Sciences and Engineering Research Council (NSERC) of Canada, the Canada Research Chair program, Canada Foundation for Innovation (CFI), the Manitoba Research and Innovation Fund, and the University of Manitoba
- Compute Canada (Grex) and local cluster (Ruthenium)

Thanks for your attention!