BPU11 CONGRESS, 28 August – 1 September 2022, Belgrade, Serbia

Graphene's striped moiré acting as a switchman for metal adatoms


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When a superlattice is seen in graphene, that’s a moiré

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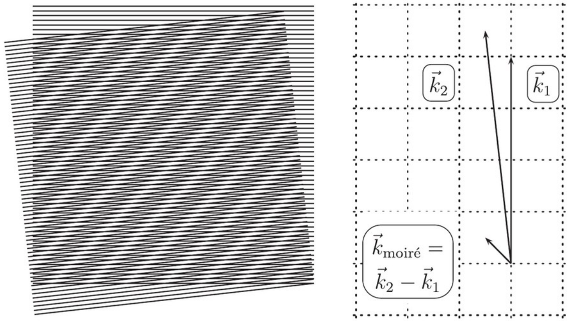
Moiré is a superposition of two lattices generating a third one



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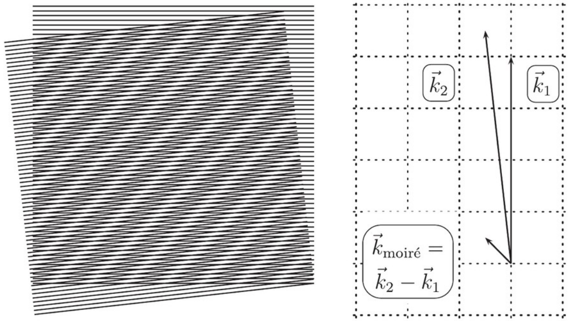
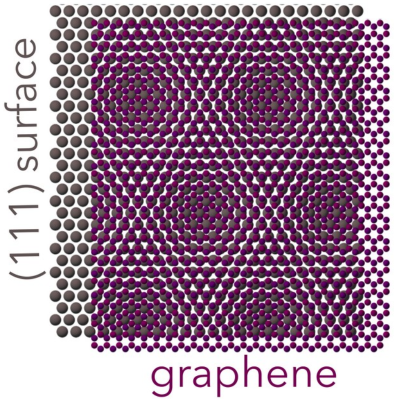


Graphene (G) on metal surfaces

lattice mismatch or misalignment to a substrate leads to a moiré pattern



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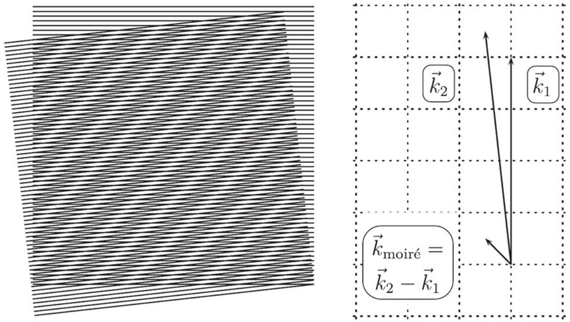
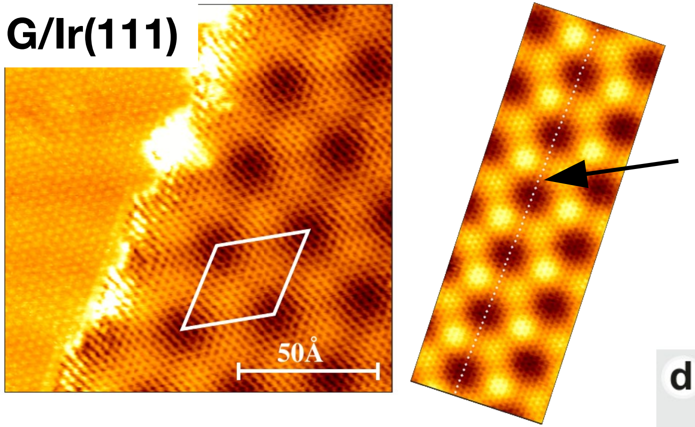


graphene forms moiré on Rh(111), Pd(111), Ir(111), Cu(111), Ru(0001) → sixfold substrates

N'Diaye *et al*, New J. Phys. **10**, 043033 (2008)


G/Ir(111)

small white dots are centers of G's hexagons

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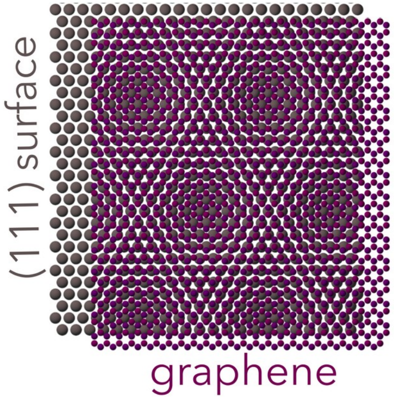
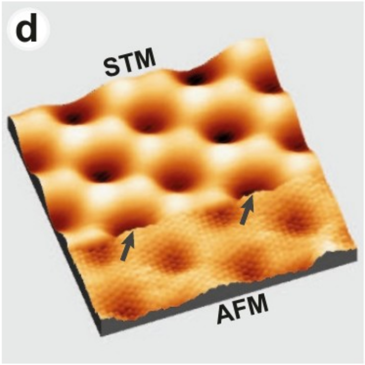


Combined STM/AFM scan of (10x10) G on (9x9) Ir(111)

Voloshina *et al*, Sci. Rep. **3**, 1072 (2013)



What’s the use of graphene’s moiré?

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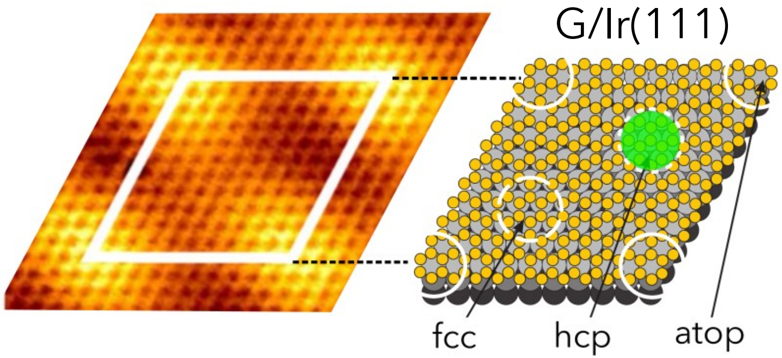
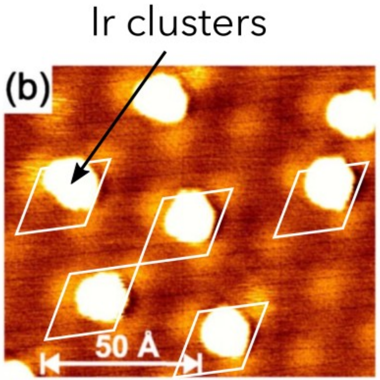
template for fabricating a highly ordered array of Ir clusters on G/Ir(111)



N'Diaye et al, *Phys. Rev. Lett.* **97**, 215501 (2006)

Pan et al, *Appl. Phys. Lett.* **95**, 093106 (2009) → Pt



$\Theta = 0.02$ ML

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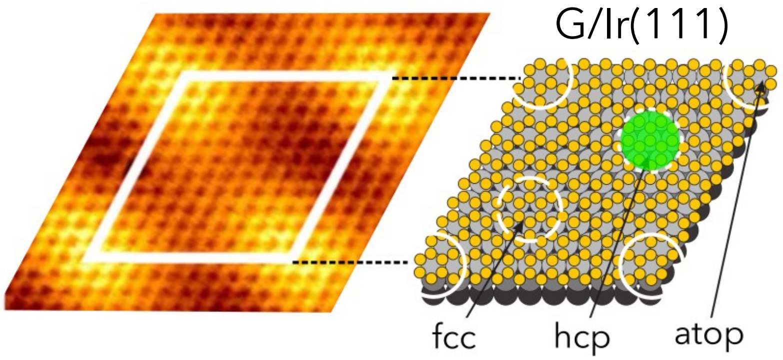

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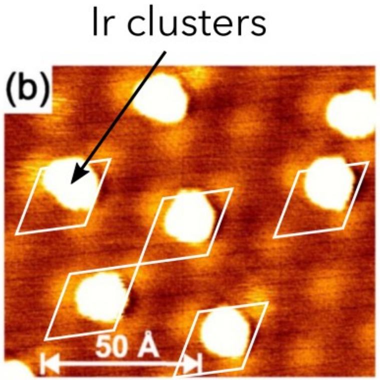

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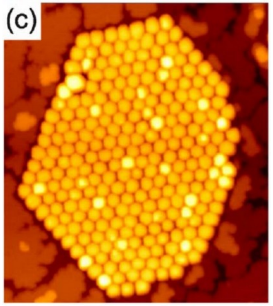

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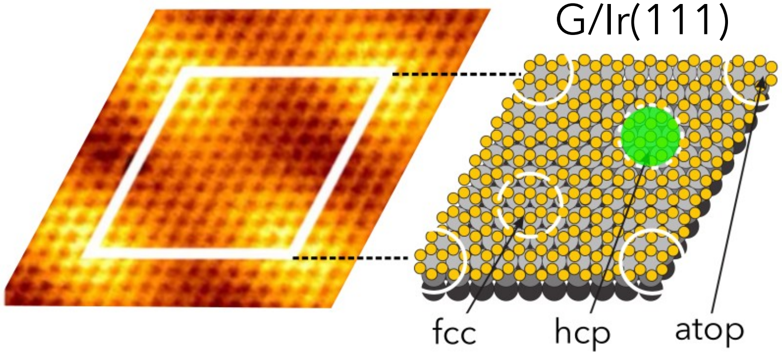

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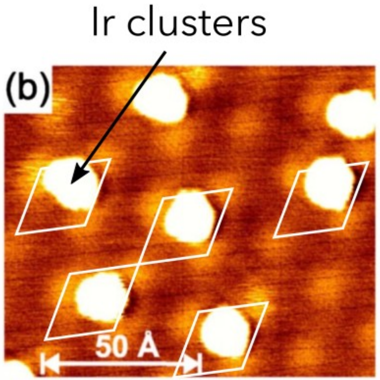

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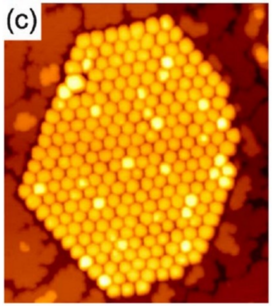

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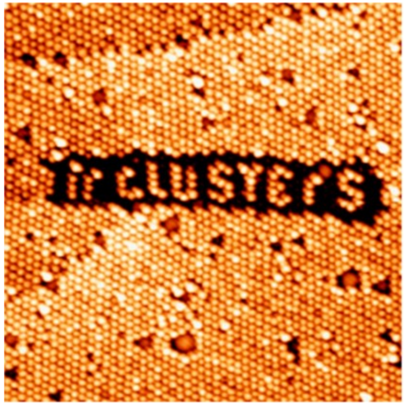
Nanowritting on G/Ru(0001)



stable for 24h+ at room temp.

Diez-Albar et al, *J. Phys. Chem. C* 123, 5525 (2019)

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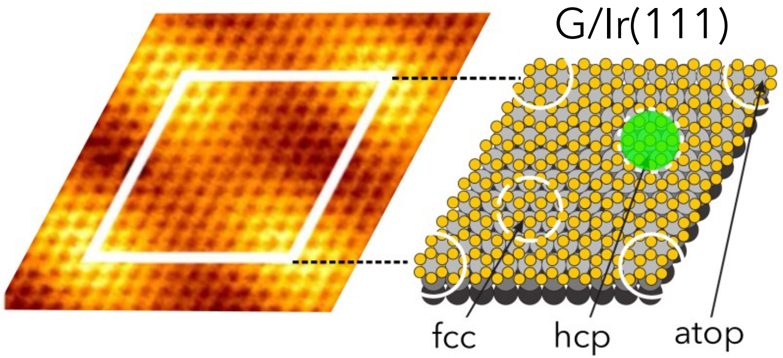

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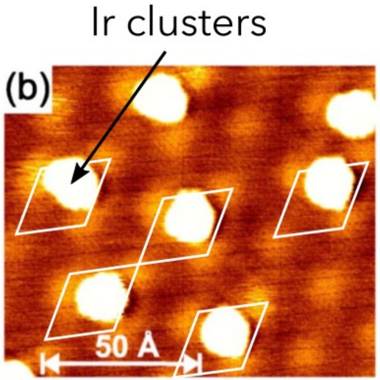

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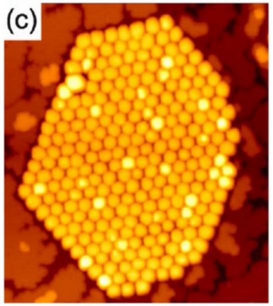

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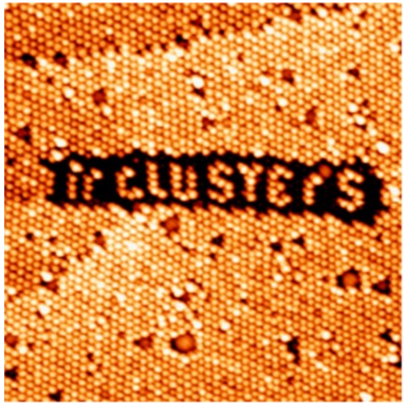

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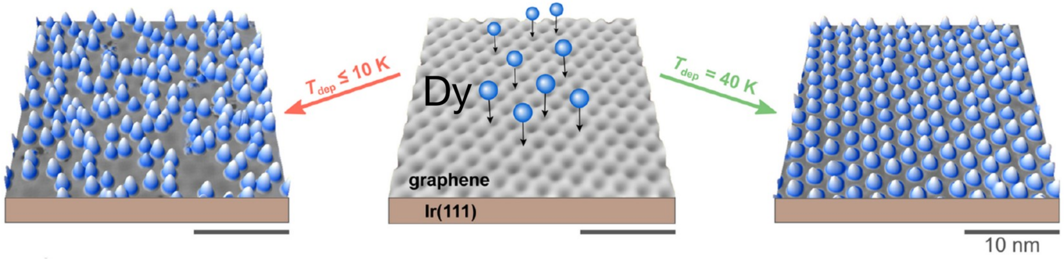
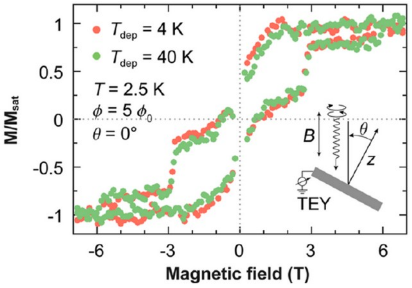
superlattice of **single-atom magnets**



Baltic et al, *Nano Lett.* **16**, 7610 (2016)



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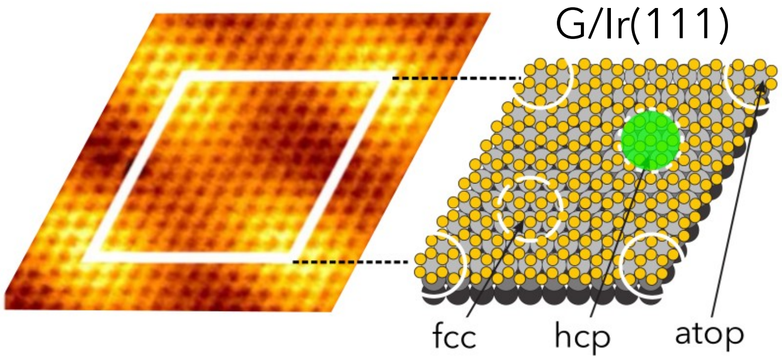

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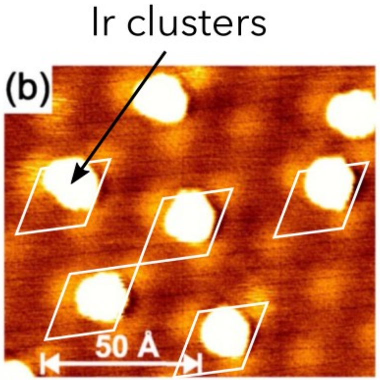

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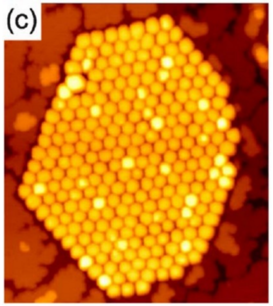

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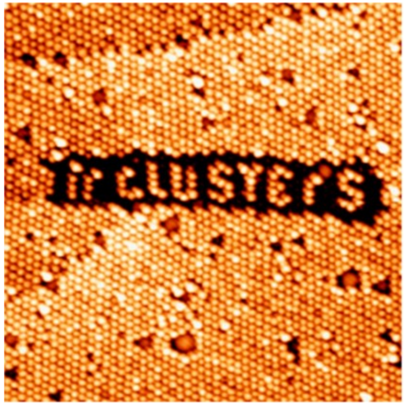

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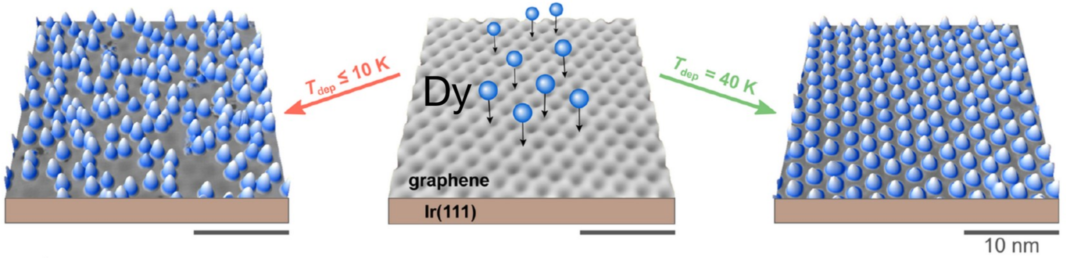

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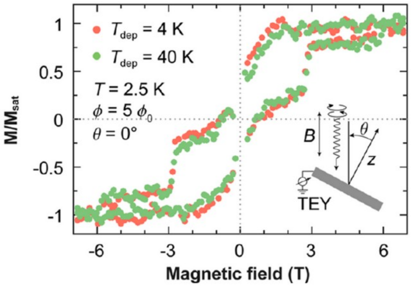

Can G form moiré other than the hexagonal network?

YES! A striped moiré can occur!

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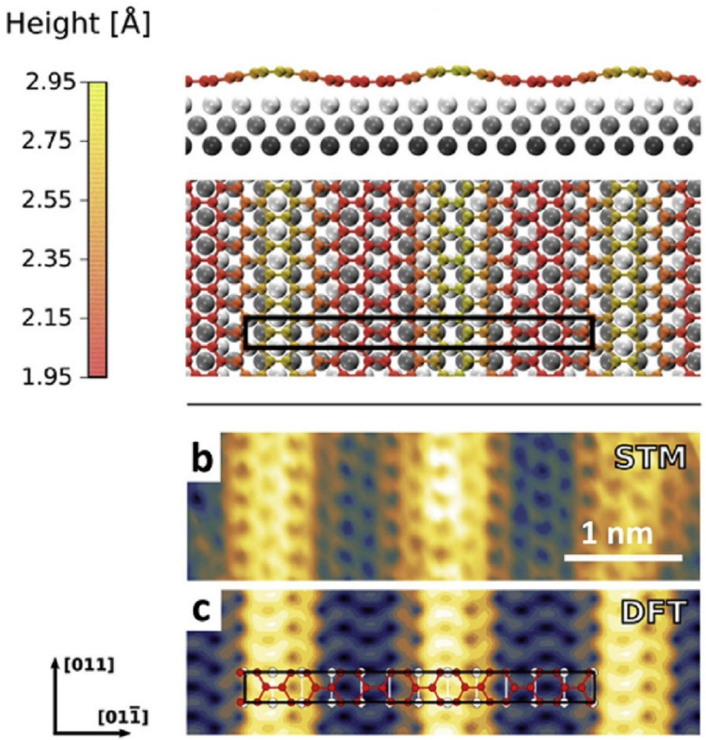
G forms **striped moiré** when grown on a **symmetry-mismatched substrate**, such as Ni(100) which has a square lattice



Zou et al, *Carbon* **130**, 441 (2018)

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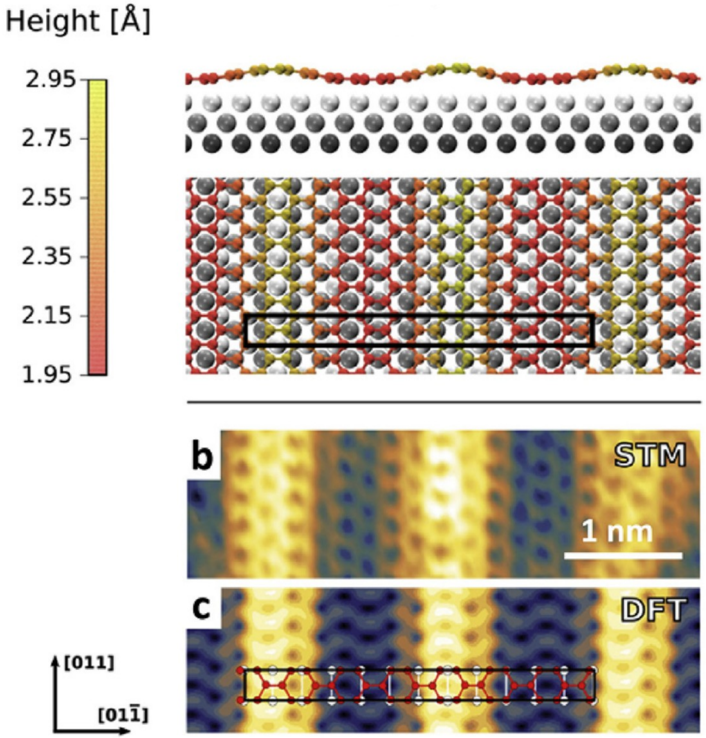
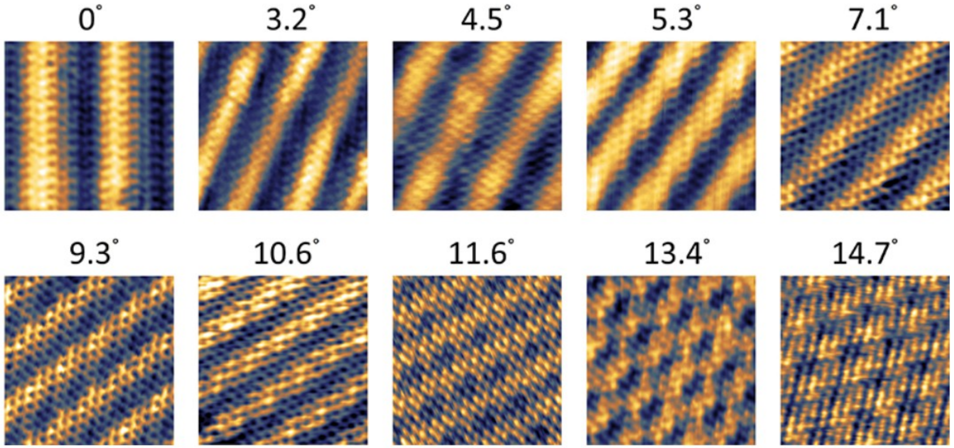


Zou et al, *Carbon* **130**, 441 (2018)

stripes → rhombic network when G is rotated



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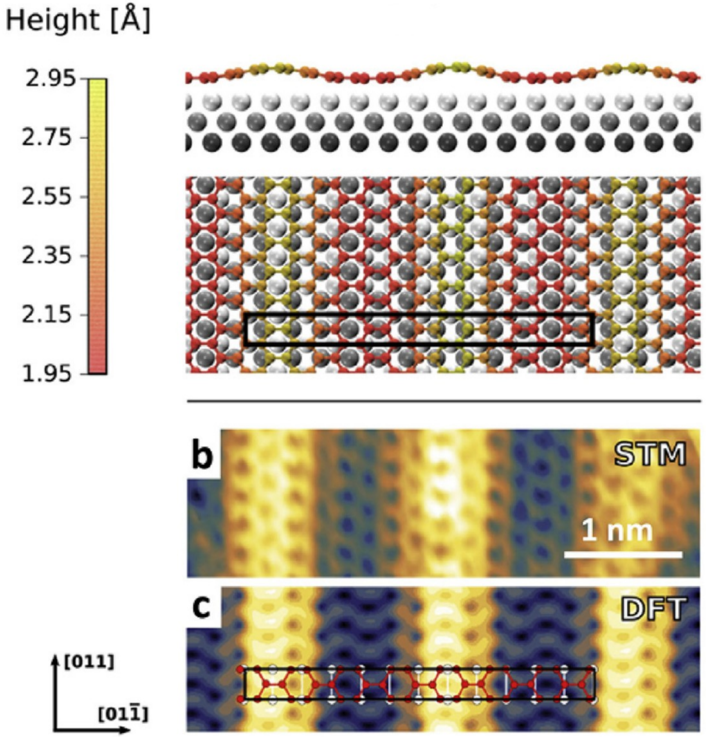

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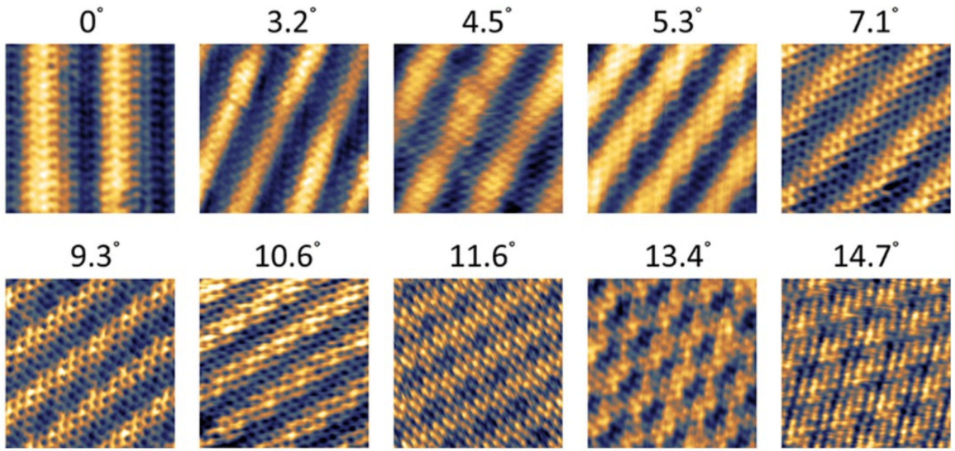
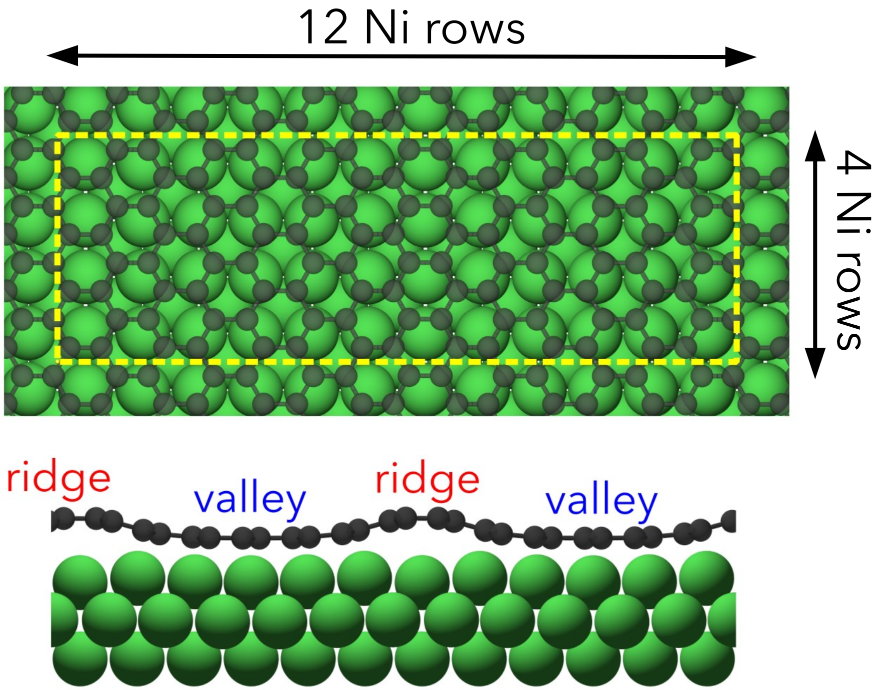


Zou et al, *J. Phys. Chem. C* **124**, 25308 (2020)

"… striped moires could induce periodically modulated electrostatic field or 1D charge accumulation/depletion, which could be exploited for tuning the band structure of G, selective modification of its chemical activity, and patterned preparation of 1D nanostructures."

Computational approach and modeling the G/Ni(100)



4x12 supercell with 256 atoms
3 Ni layers, bottom layer fixed
perfect matching of lattices

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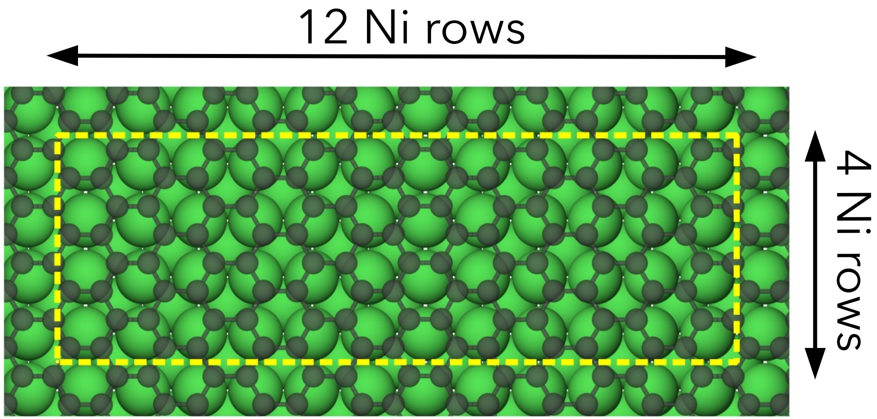

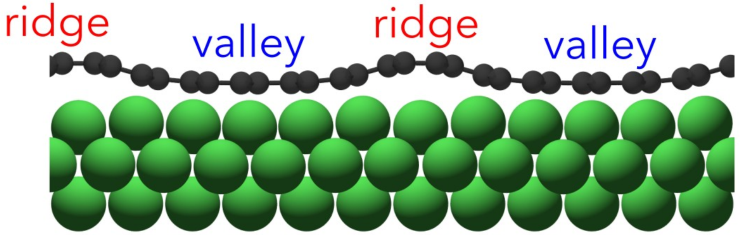

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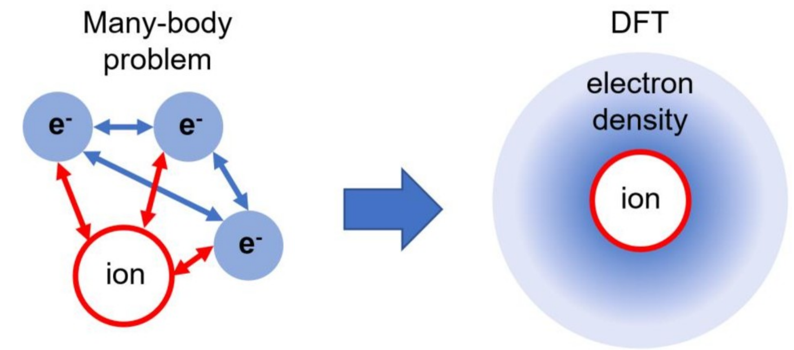
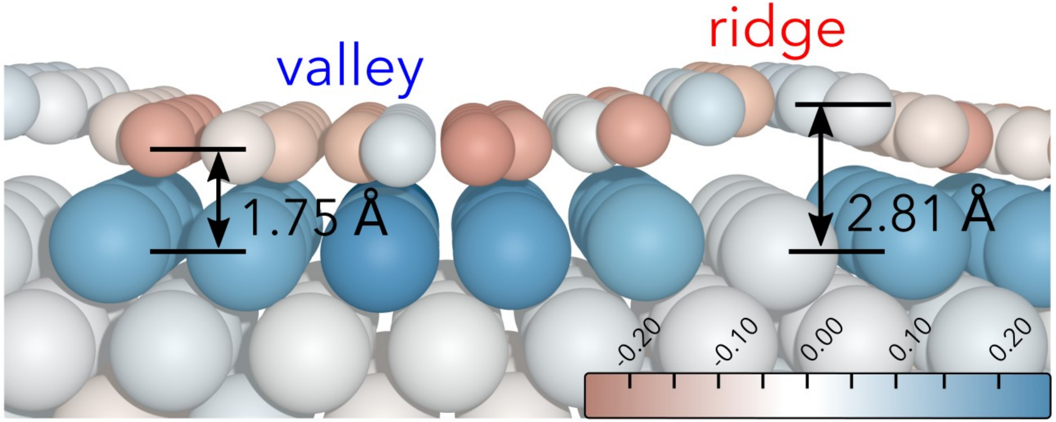
Density functional theory (DFT) calculations



Exchange and correlation in electron gas are described using **PBE** and **vdW-DF2** correction

Charge redistribution upon G adsorption

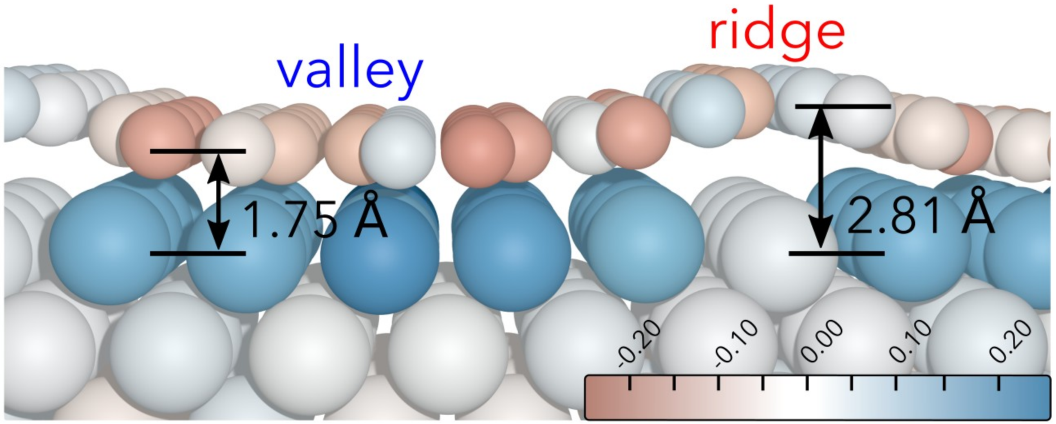
Charge redistribution upon G adsorption



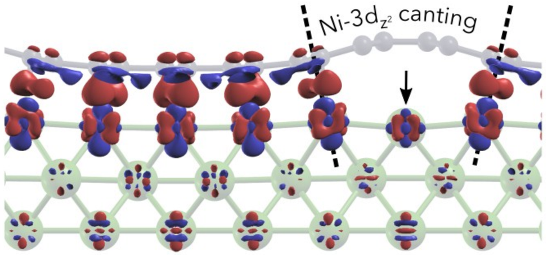
G is n-doped

S. Stavrić, V. Chesnyak, S. del Puppo, C. Africh, M. Peressi, *in preparation*

Charge redistribution upon G adsorption



induced electron density



G is n-doped

Ni atoms below the valley donate electrons (e^-) to G

Ni atoms below the ridge are not influenced by G adsorption

S. Stavrić, V. Chesnyak, S. del Puppo, C. Africh, M. Peressi, *in preparation*

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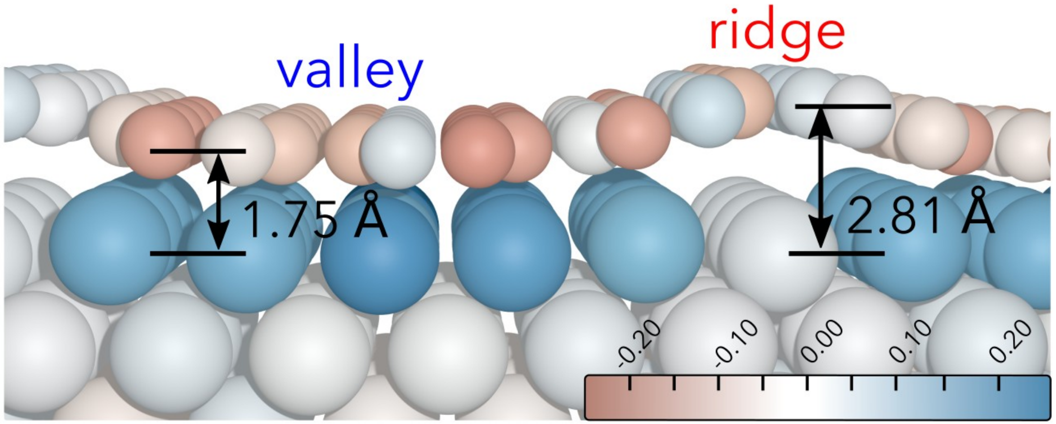

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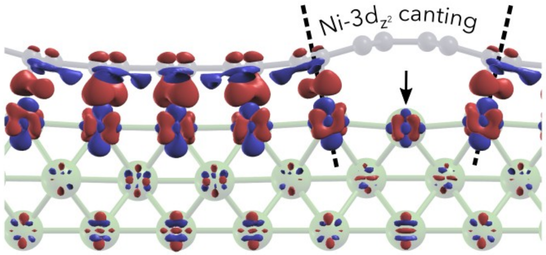
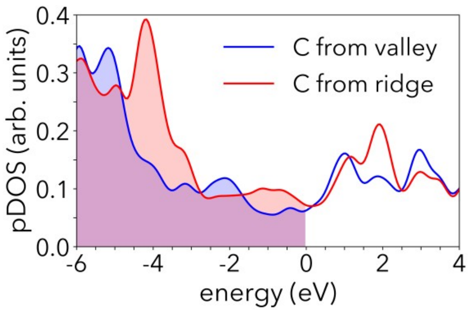


density of states



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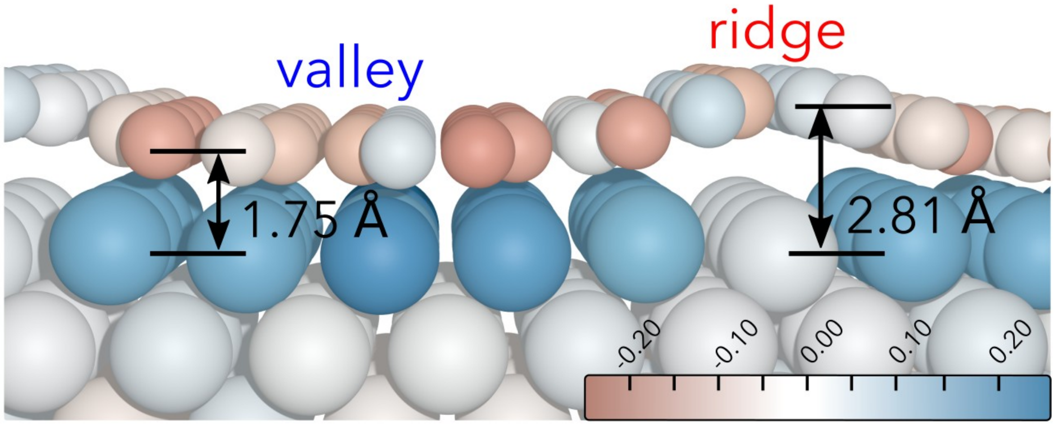
Ni atoms below the valley donate electrons (e^-) to G

Ni atoms below the ridge are not influenced by G adsorption

the chemysorption of the valley and physisorption of the ridge

Charge redistribution upon G adsorption



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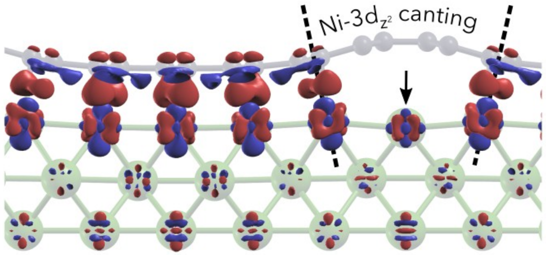

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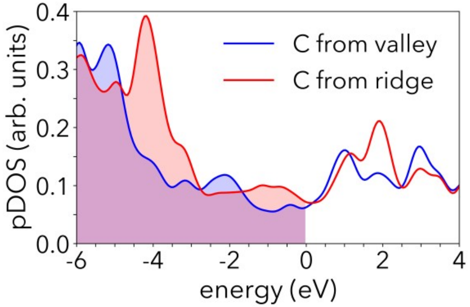


G is n-doped

Ni atoms below the valley donate electrons (e^-) to G

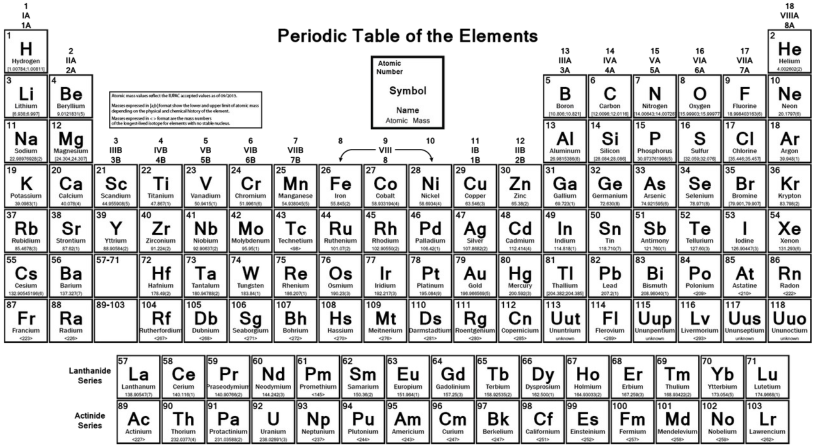
Ni atoms below the ridge are not influenced by G adsorption

the chemysorption of the valley and physisorption of the ridge

G's valleys are flat whereas ridges are curved though not sufficiently to influence G's reactivity

S. Stavrić, V. Chesnyak, S. del Puppo, C. Africh, M. Peressi, *in preparation*

Reactivity of valleys and ridges



Periodic Table of the Elements

Atomic Number
Symbol
Name
Atomic Mass

Atomic mass values reflect the IUPAC accepted values as of 09/2013.

Masses expressed in [a;b] format show the lower and upper limit of atomic mass depending on the physical and chemical history of the element.

Masses expressed in < > format are the mass numbers of the longest-lived isotope for elements with no stable nucleus.

1 IA 1A	2 IIA 2A	3 IIIB 3B	4 IVB 4B	5 VB 5B	6 VIB 6B	7 VIIB 7B	8	9 VIII 8	10	11 IB 1B	12 IIB 2B	13 IIIA 3A	14 IVA 4A	15 VA 5A	16 VIA 6A	17 VIIA 7A	18 VIIIA 8A
1 H Hydrogen [1.00784;1.00811]																	2 He Helium 4.002602(2)
3 Li Lithium [6.938;6.997]	4 Be Beryllium 9.0121831(5)											5 B Boron [10.806;10.821]	6 C Carbon [12.0096;12.0116]	7 N Nitrogen [14.00643;14.00728]	8 O Oxygen [15.99903;15.99977]	9 F Fluorine 18.998403163(6)	10 Ne Neon 20.1797(6)
11 Na Sodium 22.98976928(2)	12 Mg Magnesium [24.304,24.307]											13 Al Aluminum 26.9815385(8)	14 Si Silicon [28.084;28.086]	15 P Phosphorus 30.973761998(5)	16 S Sulfur [32.059;32.076]	17 Cl Chlorine [35.446;35.457]	18 Ar Argon 39.948(1)
19 K Potassium 39.0983(1)	20 Ca Calcium 40.078(4)	21 Sc Scandium 44.955908(5)	22 Ti Titanium 47.867(1)	23 V Vanadium 50.9415(1)	24 Cr Chromium 51.9961(6)	25 Mn Manganese 54.938045(5)	26 Fe Iron 55.845(2)	27 Co Cobalt 58.933194(4)	28 Ni Nickel 58.6934(4)	29 Cu Copper 63.546(3)	30 Zn Zinc 65.38(2)	31 Ga Gallium 69.723(1)	32 Ge Germanium 72.630(8)	33 As Arsenic 74.921595(6)	34 Se Selenium 78.971(8)	35 Br Bromine [79.901,79.907]	36 Kr Krypton 83.798(2)
37 Rb Rubidium 85.4678(3)	38 Sr Strontium 87.62(1)	39 Y Yttrium 88.90584(2)	40 Zr Zirconium 91.224(2)	41 Nb Niobium 92.90637(2)	42 Mo Molybdenum 95.95(1)	43 Tc Technetium <98>	44 Ru Ruthenium 101.07(2)	45 Rh Rhodium 102.90550(2)	46 Pd Palladium 106.42(1)	47 Ag Silver 107.8682(2)	48 Cd Cadmium 112.414(4)	49 In Indium 114.818(1)	50 Sn Tin 118.710(7)	51 Sb Antimony 121.760(1)	52 Te Tellurium 127.60(3)	53 I Iodine 126.90447(3)	54 Xe Xenon 131.293(6)
55 Cs Cesium 132.90545196(6)	56 Ba Barium 137.327(7)	57-71	72 Hf Hafnium 178.49(2)	73 Ta Tantalum 180.94788(2)	74 W Tungsten 183.84(1)	75 Re Rhenium 186.207(1)	76 Os Osmium 190.23(3)	77 Ir Iridium 192.217(3)	78 Pt Platinum 195.084(9)	79 Au Gold 196.966569(5)	80 Hg Mercury 200.592(3)	81 Tl Thallium [204.382;204.385]	82 Pb Lead 207.2(1)	83 Bi Bismuth 208.98040(1)	84 Po Polonium <209>	85 At Astatine <210>	86 Rn Radon <222>
87 Fr Francium <223>	88 Ra Radium <226>	89-103	104 Rf Rutherfordium <267>	105 Db Dubnium <268>	106 Sg Seaborgium <271>	107 Bh Bohrium <272>	108 Hs Hassium <270>	109 Mt Meitnerium <276>	110 Ds Darmstadtium <281>	111 Rg Roentgenium <280>	112 Cn Copernicium <285>	113 Uut Ununtrium unknown	114 Fl Flerovium <289>	115 Uup Ununpentium unknown	116 Lv Livermorium <293>	117 Uus Ununseptium unknown	118 Uuo Ununoctium unknown

Lanthanide Series	57 La Lanthanum 138.90547(7)	58 Ce Cerium 140.116(1)	59 Pr Praseodymium 140.90766(2)	60 Nd Neodymium 144.242(3)	61 Pm Promethium <145>	62 Sm Samarium 150.36(2)	63 Eu Europium 151.964(1)	64 Gd Gadolinium 157.25(3)	65 Tb Terbium 158.92535(2)	66 Dy Dysprosium 162.500(1)	67 Ho Holmium 164.93033(2)	68 Er Erbium 167.259(3)	69 Tm Thulium 168.93422(2)	70 Yb Ytterbium 173.054(5)	71 Lu Lutetium 174.9668(1)
Actinide Series	89 Ac Actinium <227>	90 Th Thorium 232.0377(4)	91 Pa Protactinium 231.03588(2)	92 U Uranium 238.02891(3)	93 Np Neptunium <237>	94 Pu Plutonium <244>	95 Am Americium <243>	96 Cm Curium <247>	97 Bk Berkelium <247>	98 Cf Californium <251>	99 Es Einsteinium <252>	100 Fm Fermium <257>	101 Md Mendelevium <258>	102 No Nobelium <259>	103 Lr Lawrencium <262>

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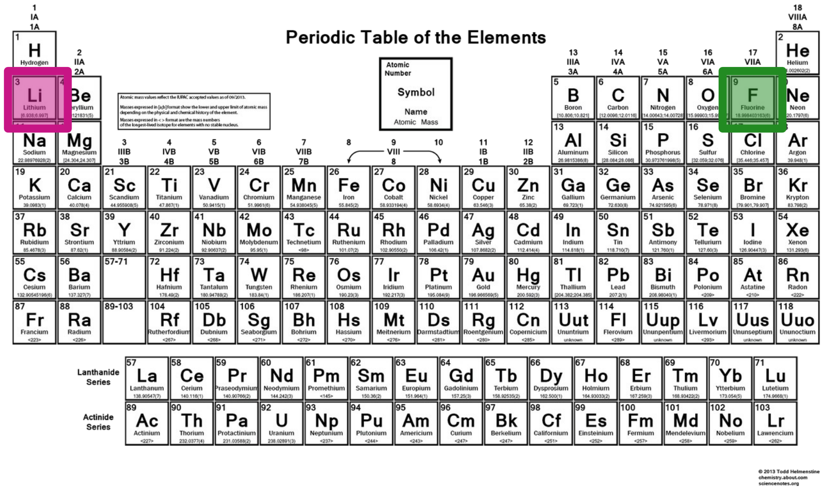
Reactivity of valleys and ridges



Periodic Table of the Elements

1 IA 1A	2 IIA 2A	3 IIIB 3B	4 IVB 4B	5 VB 5B	6 VIB 6B	7 VIIB 7B	8 VIII 8	9 VIII 8	10 VIII 8	11 IB 1B	12 IIB 2B	13 IIIA 3A	14 IVA 4A	15 VA 5A	16 VIA 6A	17 VIIA 7A	18 VIIIA 8A
1 H Hydrogen																	2 He Helium
3 Li Lithium	4 Be Beryllium											5 B Boron	6 C Carbon	7 N Nitrogen	8 O Oxygen	9 F Fluorine	10 Ne Neon
11 Na Sodium	12 Mg Magnesium											13 Al Aluminum	14 Si Silicon	15 P Phosphorus	16 S Sulfur	17 Cl Chlorine	18 Ar Argon
19 K Potassium	20 Ca Calcium	21 Sc Scandium	22 Ti Titanium	23 V Vanadium	24 Cr Chromium	25 Mn Manganese	26 Fe Iron	27 Co Cobalt	28 Ni Nickel	29 Cu Copper	30 Zn Zinc	31 Ga Gallium	32 Ge Germanium	33 As Arsenic	34 Se Selenium	35 Br Bromine	36 Kr Krypton
37 Rb Rubidium	38 Sr Strontium	39 Y Yttrium	40 Zr Zirconium	41 Nb Niobium	42 Mo Molybdenum	43 Tc Technetium	44 Ru Ruthenium	45 Rh Rhodium	46 Pd Palladium	47 Ag Silver	48 Cd Cadmium	49 In Indium	50 Sn Tin	51 Sb Antimony	52 Te Tellurium	53 I Iodine	54 Xe Xenon
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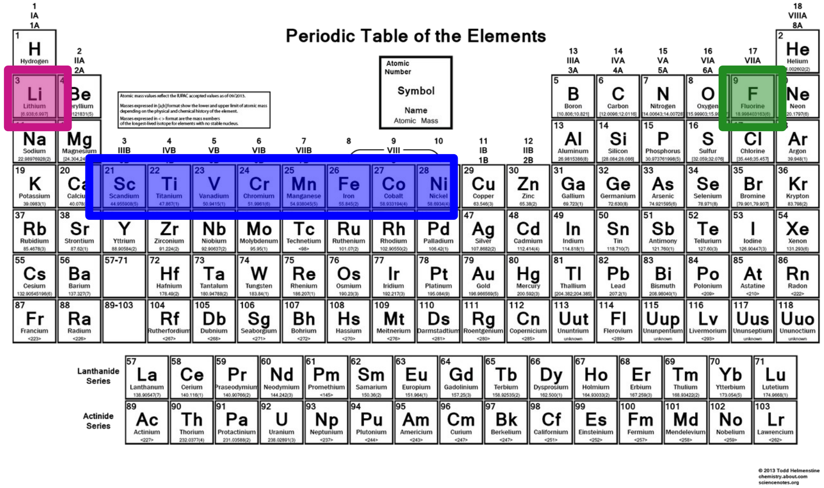
Periodic Table of the Elements

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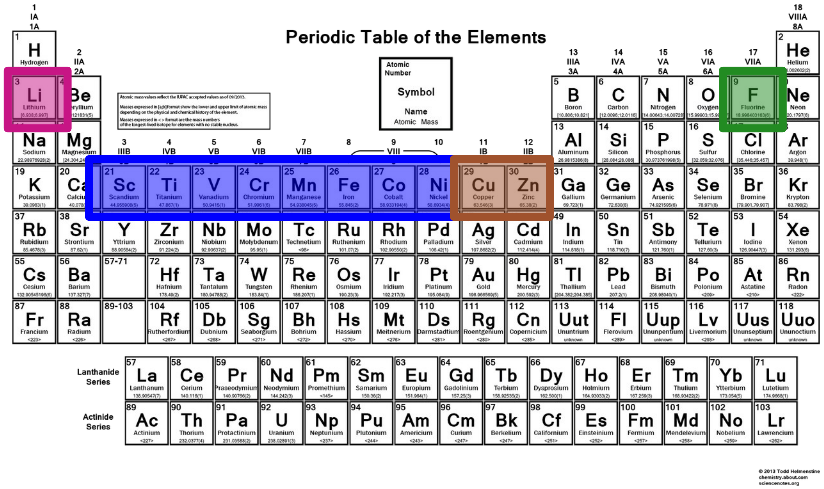

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11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
55 Cs	56 Ba	57-71	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
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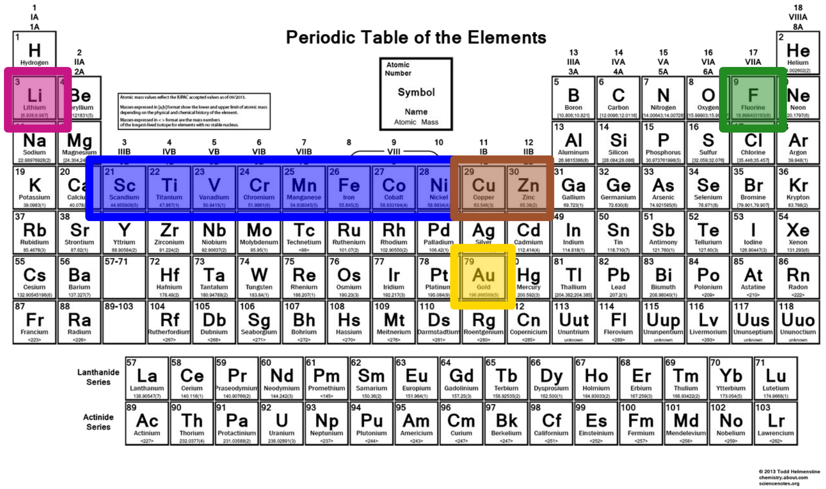

Periodic Table of the Elements

Atomic Number
Symbol
Name
Atomic Mass

Atomic mass values reflect the IUPAC accepted values as of 09/2013.

Masses expressed in [a;b] format show the lower and upper limit of atomic mass depending on the physical and chemical history of the element.

Masses expressed in < > format are the mass numbers of the longest-lived isotope for elements with no stable nucleus.

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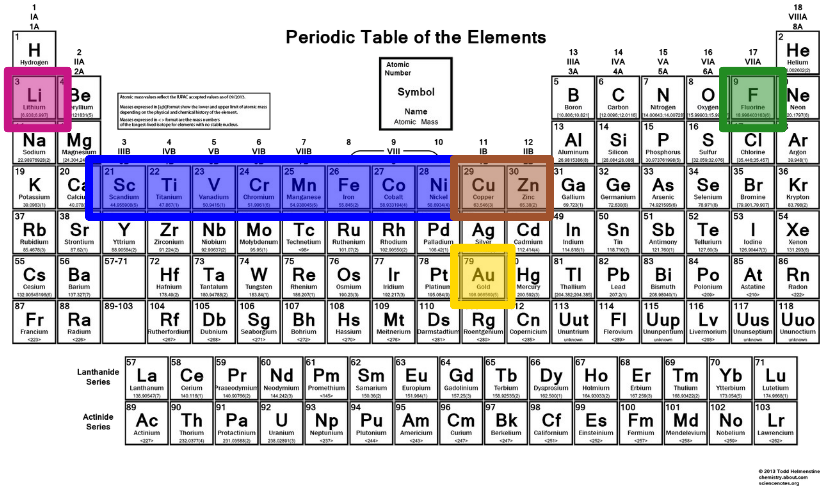
Manade et al, *Carbon* **95,** 525 (2015)

S. Stavrić, V. Chesnyak, S. del Puppo, C. Africh, M. Peressi, *in preparation*

Reactivity of valleys and ridges



$$\Delta E = E_V - E_R$$

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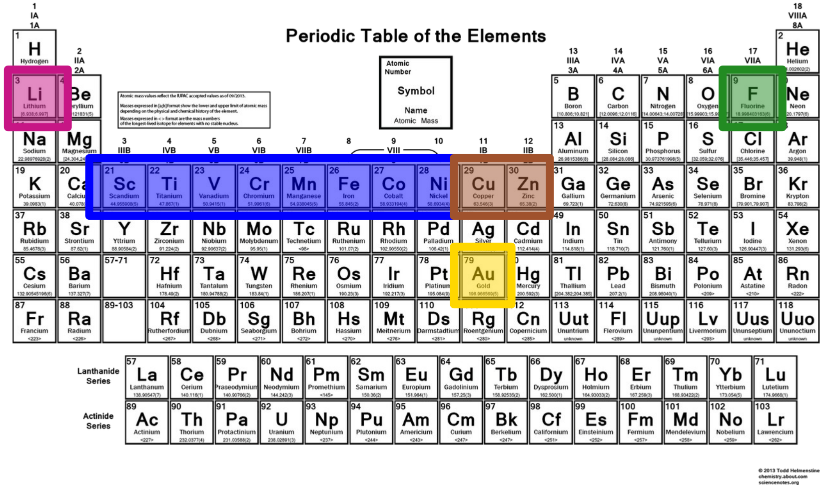

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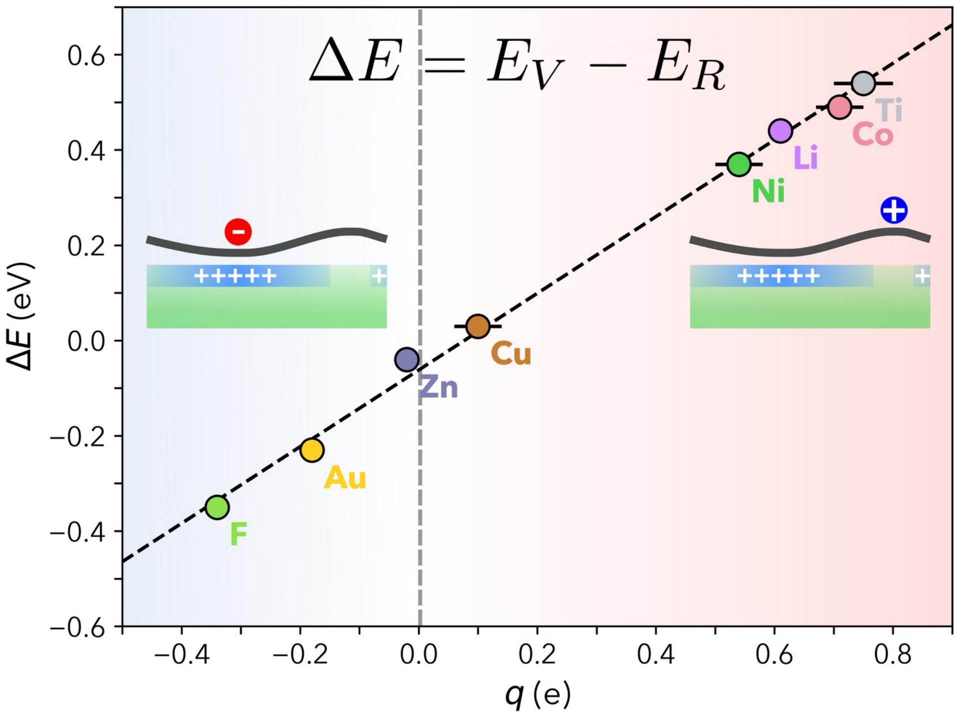

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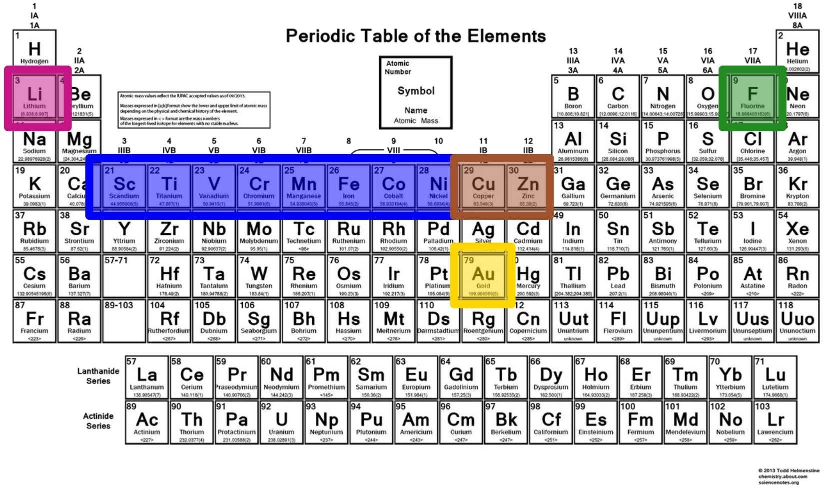

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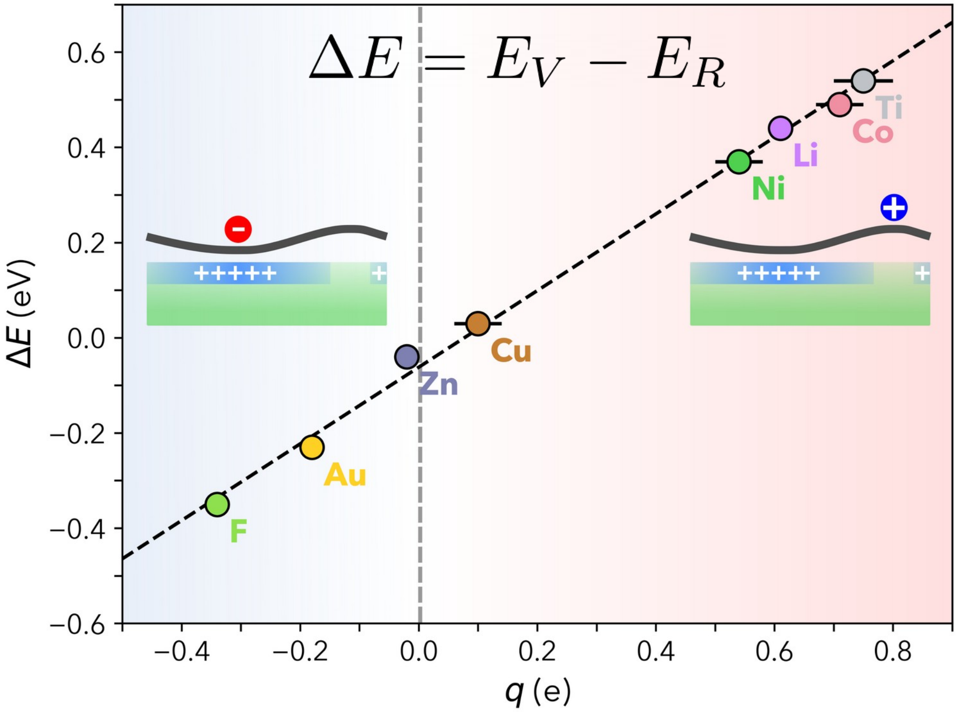

Adatom ◄—► 1st Ni layer Coulomb interaction dictates where the adatom will be adsorbed

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Mobility of Co atoms on the graphene's surface

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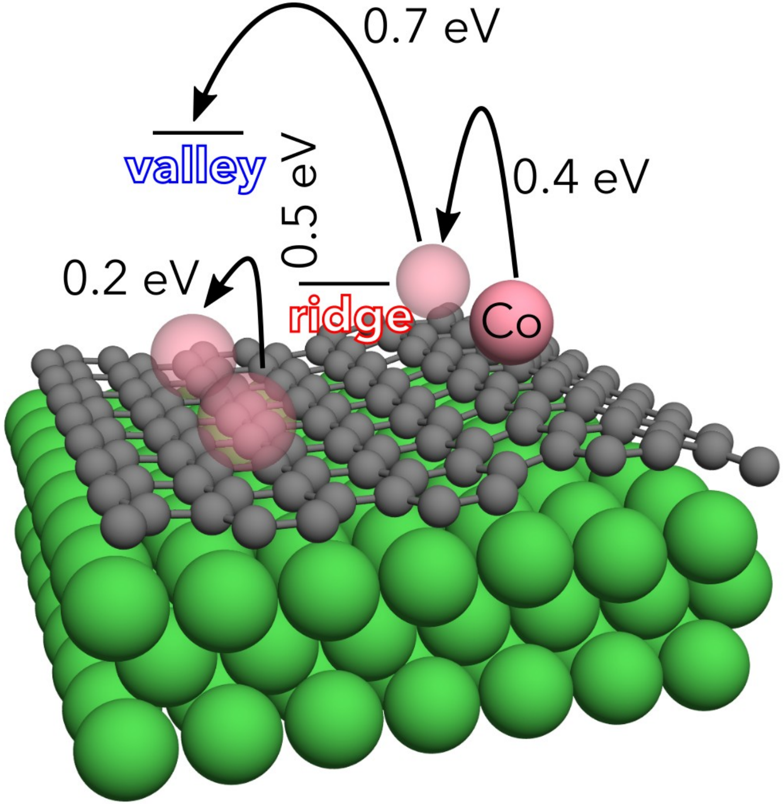
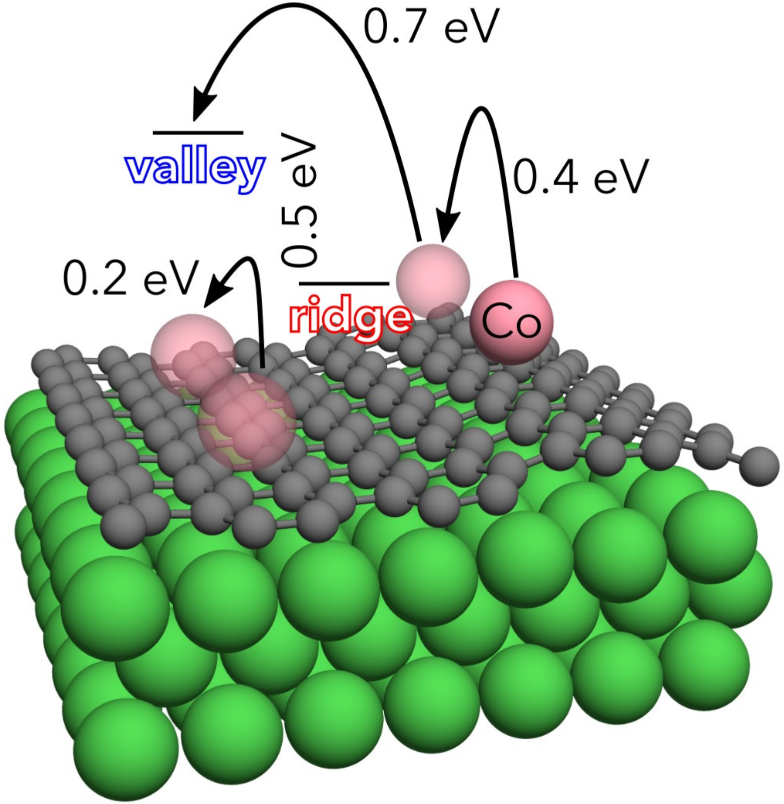


barriers calculated using the nudged elastic band method

Mobility of Co atoms on the graphene’s surface



barriers calculated using the
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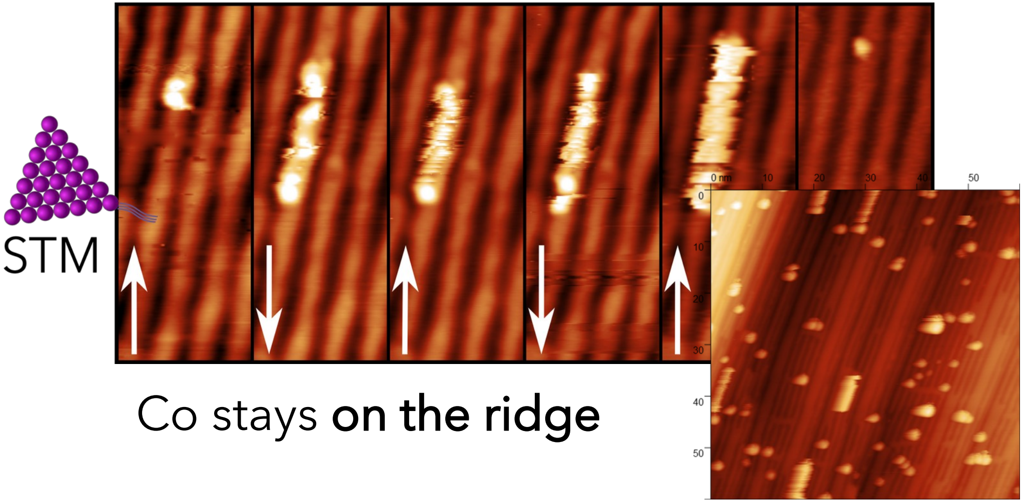
Co atom running along the ridge



Co stays **on the ridge**

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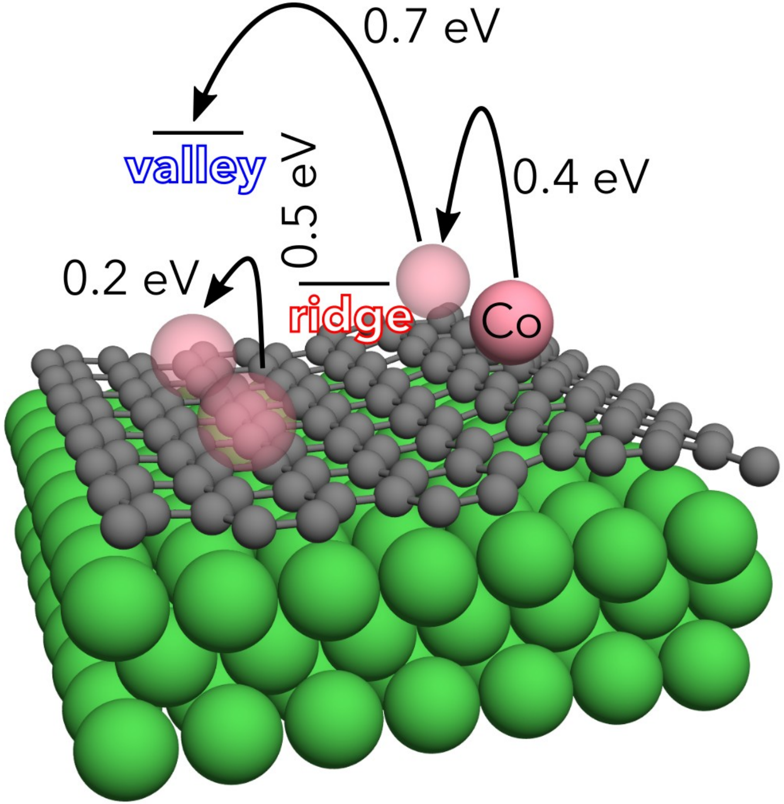

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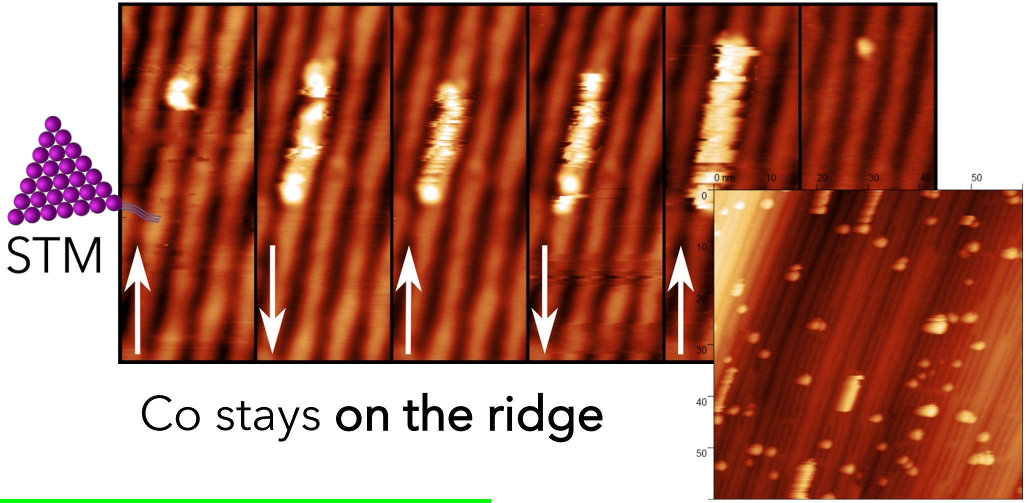

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electrostatic repulsion between Co atoms and Ni surface makes the diffusion easier along the valley

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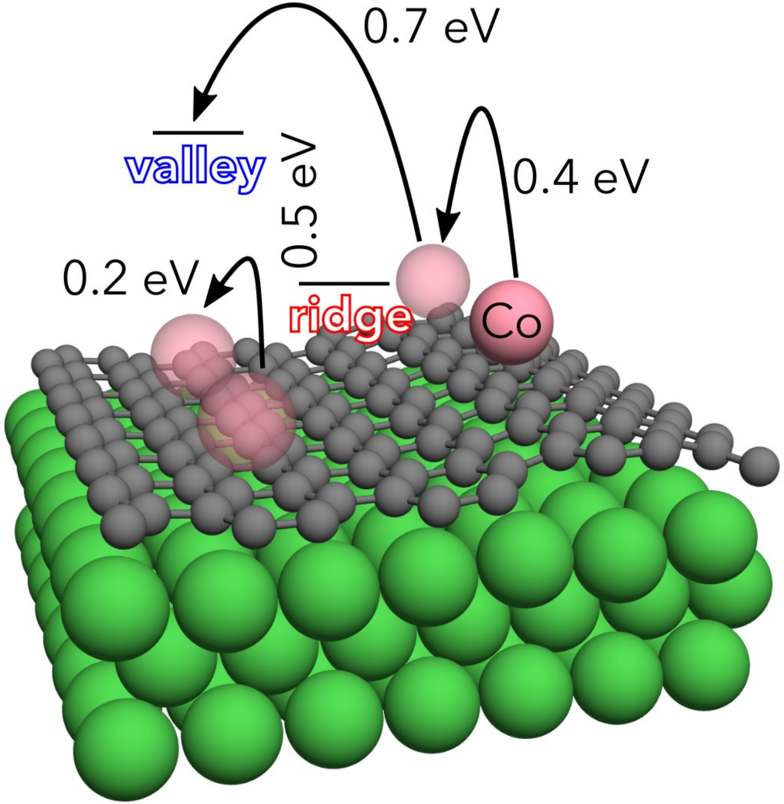

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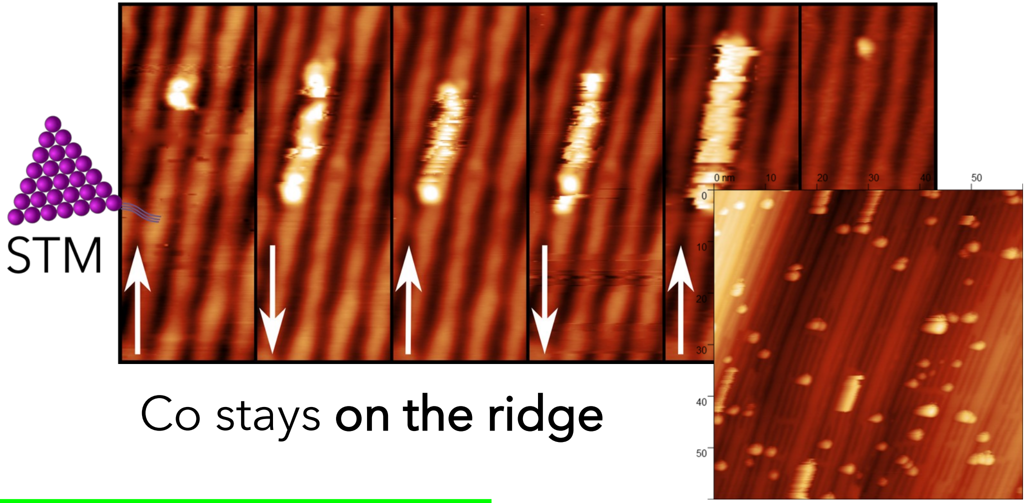

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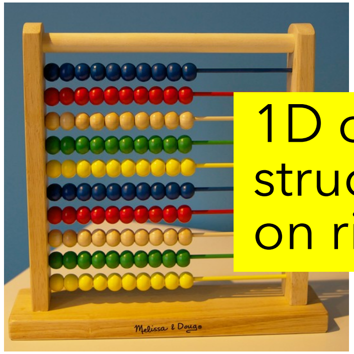

1D cobalt structures on ridges?

Co nanostructures on ridges

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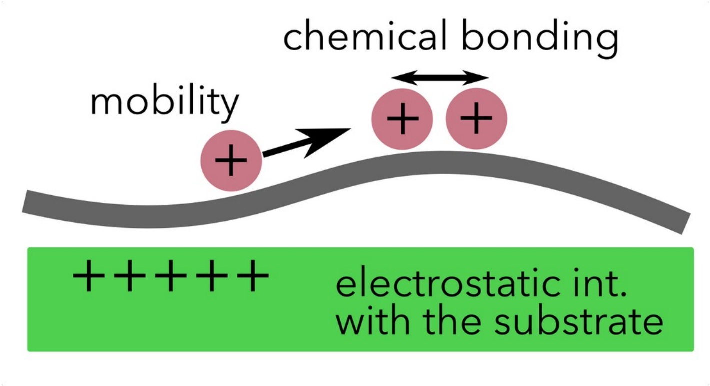
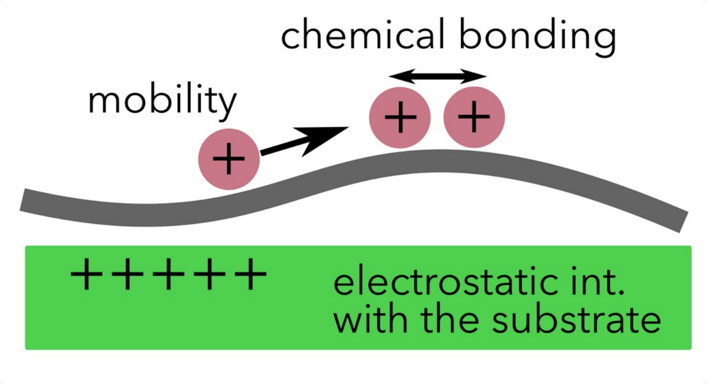
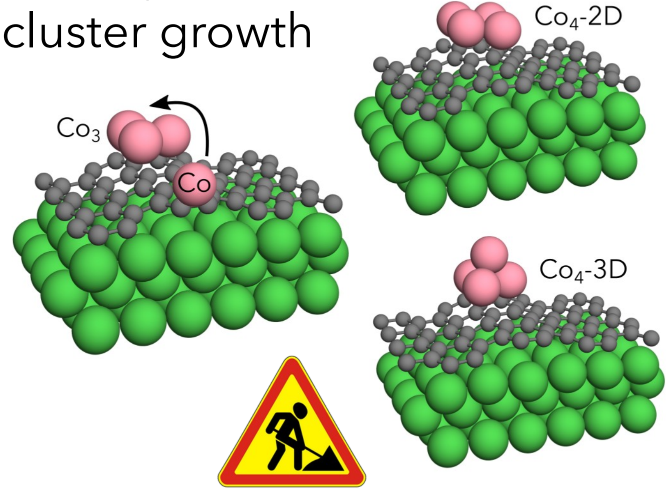


Co nanostructures on ridges



2D vs 3D
cluster growth



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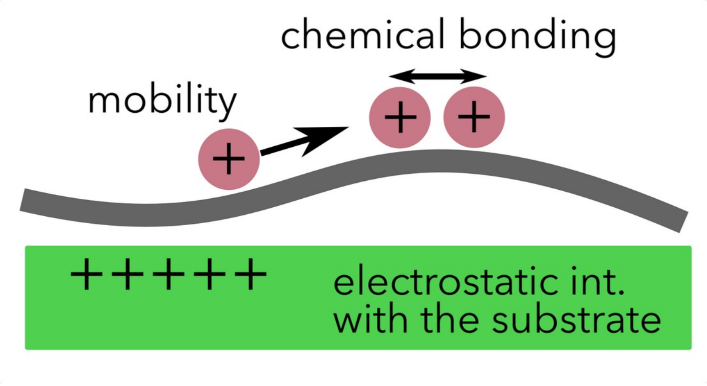

chemical bonding

mobility

+++++

electrostatic int.
with the substrate

binding energy of Co$_n$ cluster

$$E_{\mathrm{bind}} = \frac{1}{n}\Big(nE(\mathrm{Co}) + E(\mathrm{S}) - E(\mathrm{Co_n/S})\Big)$$

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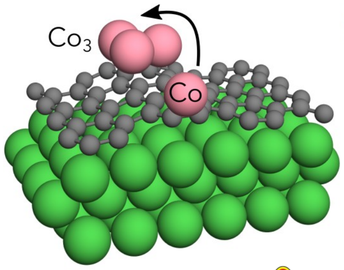

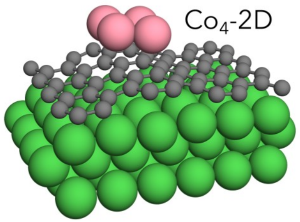

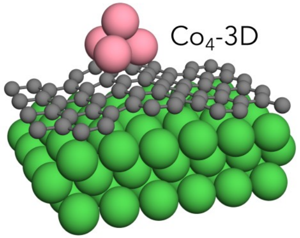

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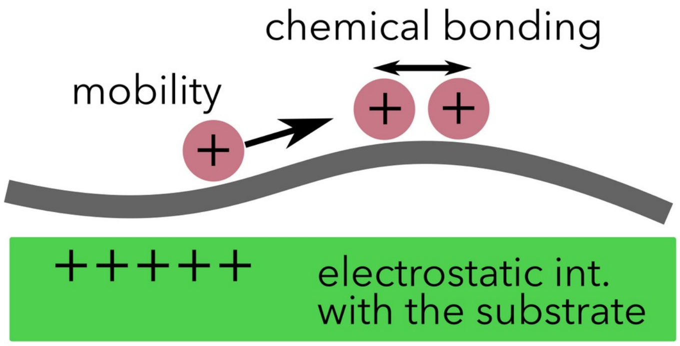

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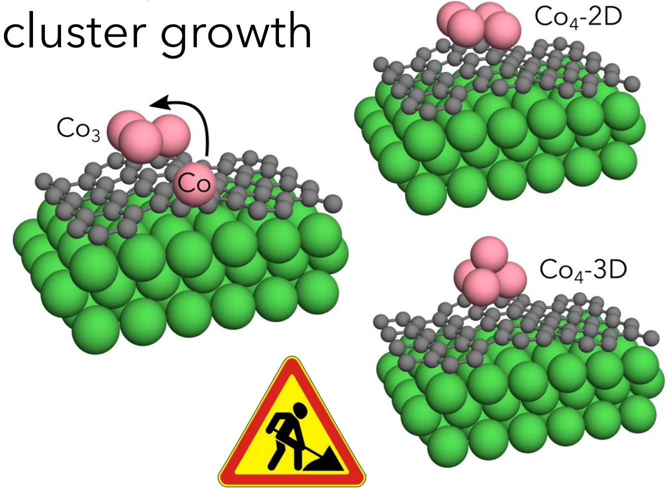

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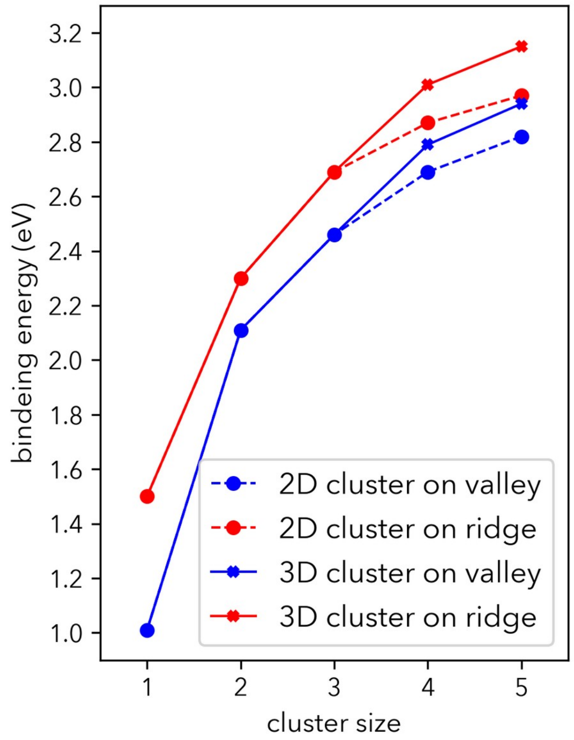

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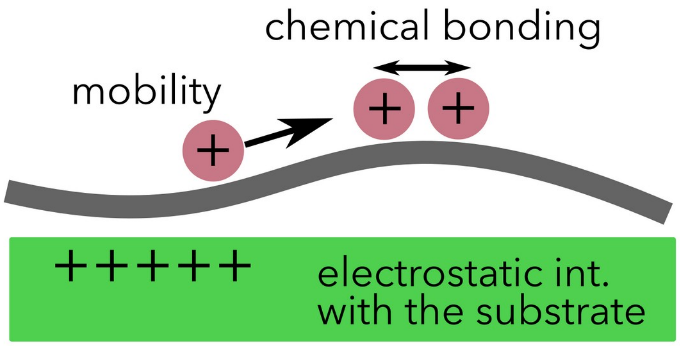

electrostatic int. with the substrate

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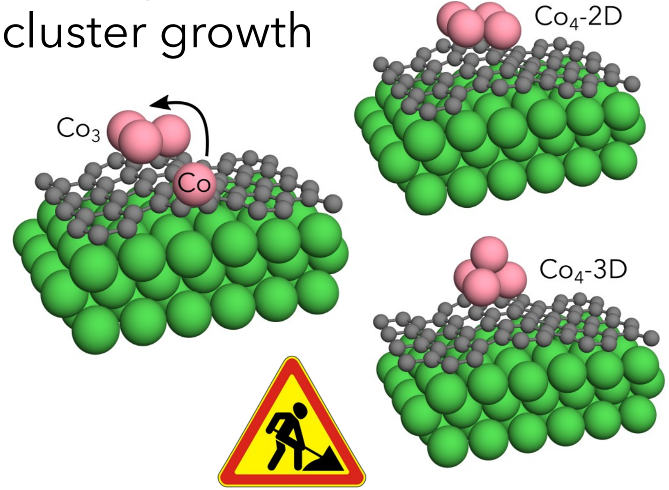

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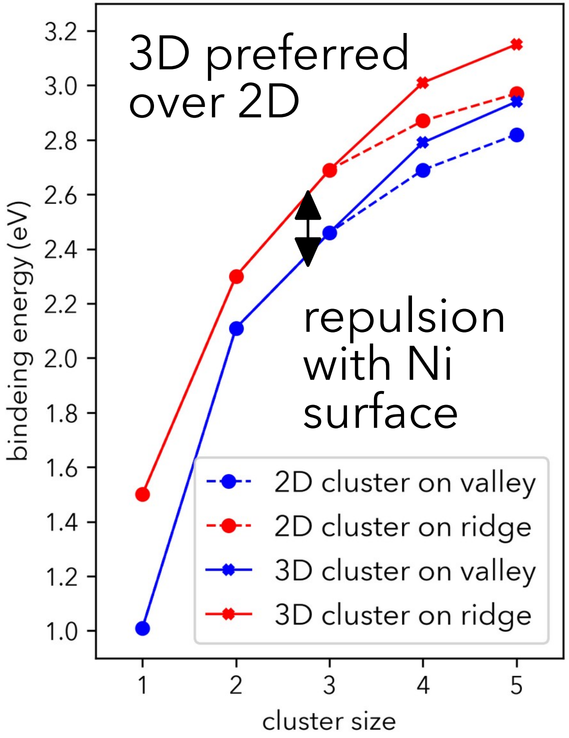

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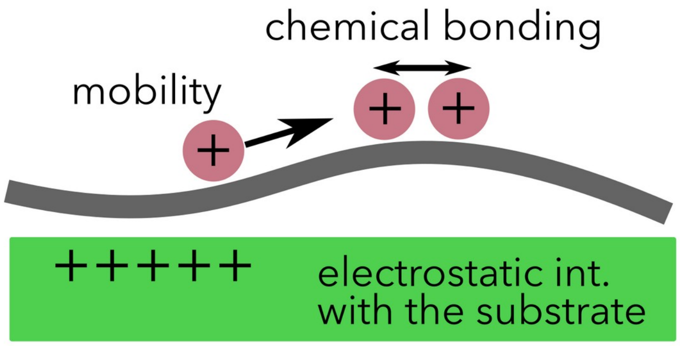

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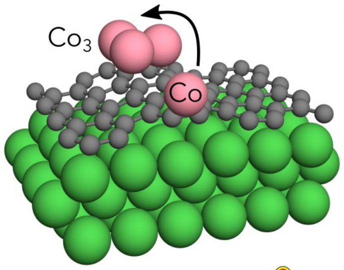
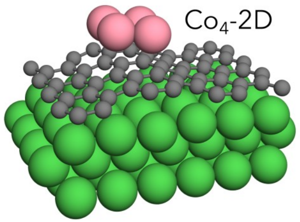
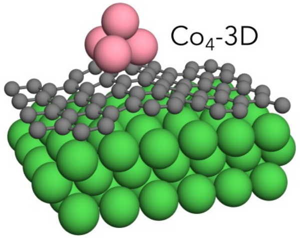
cluster growth

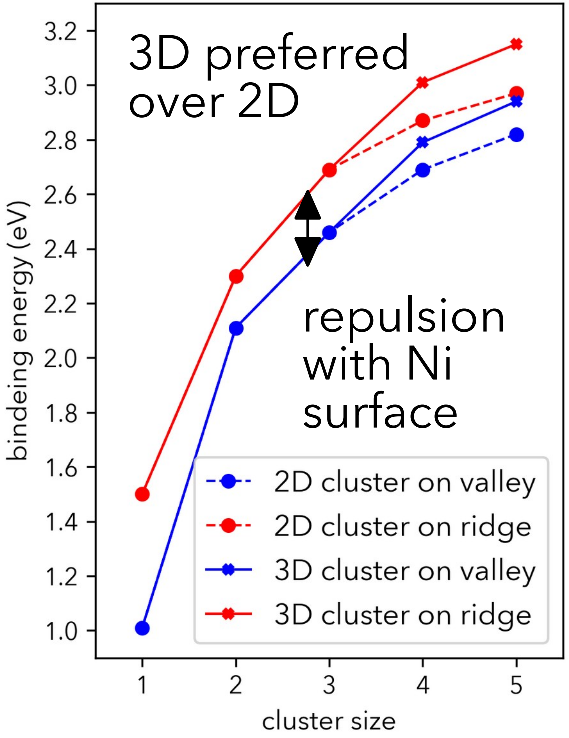




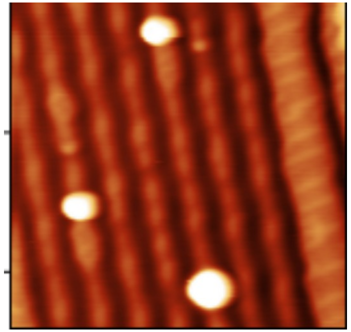


binding energy of Co$_n$ cluster

$$E_{\mathrm{bind}} = \frac{1}{n}\left(nE(\mathrm{Co}) + E(\mathrm{S}) - E(\mathrm{Co}_n/\mathrm{S})\right)$$



experiments



large roundish mostly 2-layer high clusters on ridges, that cover valleys as they grow

no evidence of 1D structures

CONCLUSIONS

Ni(100) is a fantastic substrate for the fabrication of graphene's **striped moiré**

Alternate mesh of **valleys and ridges** leads to charge redistribution in G/Ni(100)

The **electrostatic interaction** between the atom on G and the Ni surface below dictates the adsorption site of the atom

Co deposited on G/Ni(100) builds **roundish 3D nanostructures on the ridges**

Future plans:

- assess the stability in air of Co nanostructures on ridges
- try to make one-dimensional Au nanostructures on the valleys

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САНУ
СРПСКА АКАДЕМИЈА НАУКА И УМЕТНОСТИ

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Computational resources