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Chemical reactivity of pristine and defected graphene grown on nickel (111)

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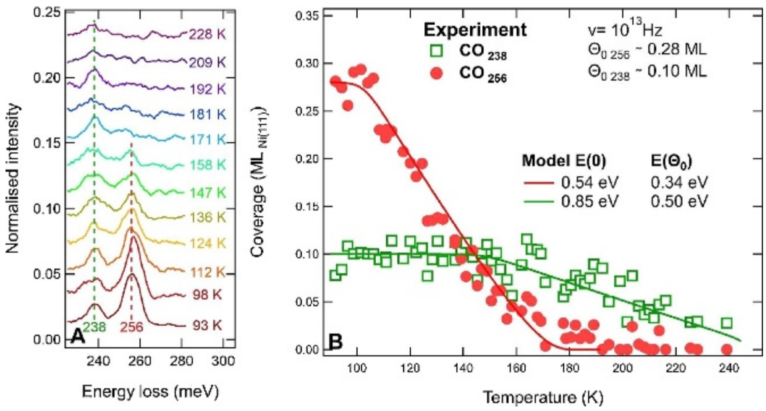
Graphene (G) is considered a promising material in many technological fields, including gas sensing and catalysis. Recently, free-standing G has been used as the sensing element for the detection of different gases [1]. The high sensitivity (ppm or better) is due to the doping induced by adsorption and depends critically on the reactant species, though the nature of the active sites is still not fully understood. It is also well established that the chemical activity of G-based materials can be modified and controlled by doping with hetero-atoms (B, N, P) or, more recently with metal atoms. Literary data suggest that chemisorption of simple gas molecules on graphene is a process involving defected or doped sites.

To clarify this issue, we performed an HREELS and XPS study on the reactivity towards CO adsorption of N-doped [2] and defected [3] G supported on Ni(111). By comparing the results obtained with those previously achieved for pristine G/Ni(111) and G/Cu samples, we succeeded in determining the role of defects introduced in the G layer in form of single vacancies or of N heteroatoms.

While the presence of single-atom vacancies opens the way towards CO adsorption at the underlying Ni(111) surface, the introduction of N atoms in the G lattice creates a new adsorption channel for weak CO chemisorption on G. A maximum adsorption energy of 0.85 eV/molecule is estimated for the latter moiety, to be compared with a value of 0.54 eV/molecule of the pristine G/Ni(111).



A): HREEL spectra recorded sequentially on the N-doped (~11%) G/Ni(111) layer exposed to 40 L of CO at T = 87 K upon warming of the sample.
B): Coverage of the two CO moieties function of sample temperature.

[1] F. Schedin et al., Nat. Mater. 6 (2007) 652. DOI: 10.1038/nmat1967
[2] G. Carraro et al, Appl. Surf. Sci. 428 (2018) 775. DOI:10.1016/j.apsusc.2017.09.194.
[3] E Celasco et al, PCCP 18, (2016) 18692. DOI: 10.1039/C6CP02999J

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