Single-layer graphene oxide architecture

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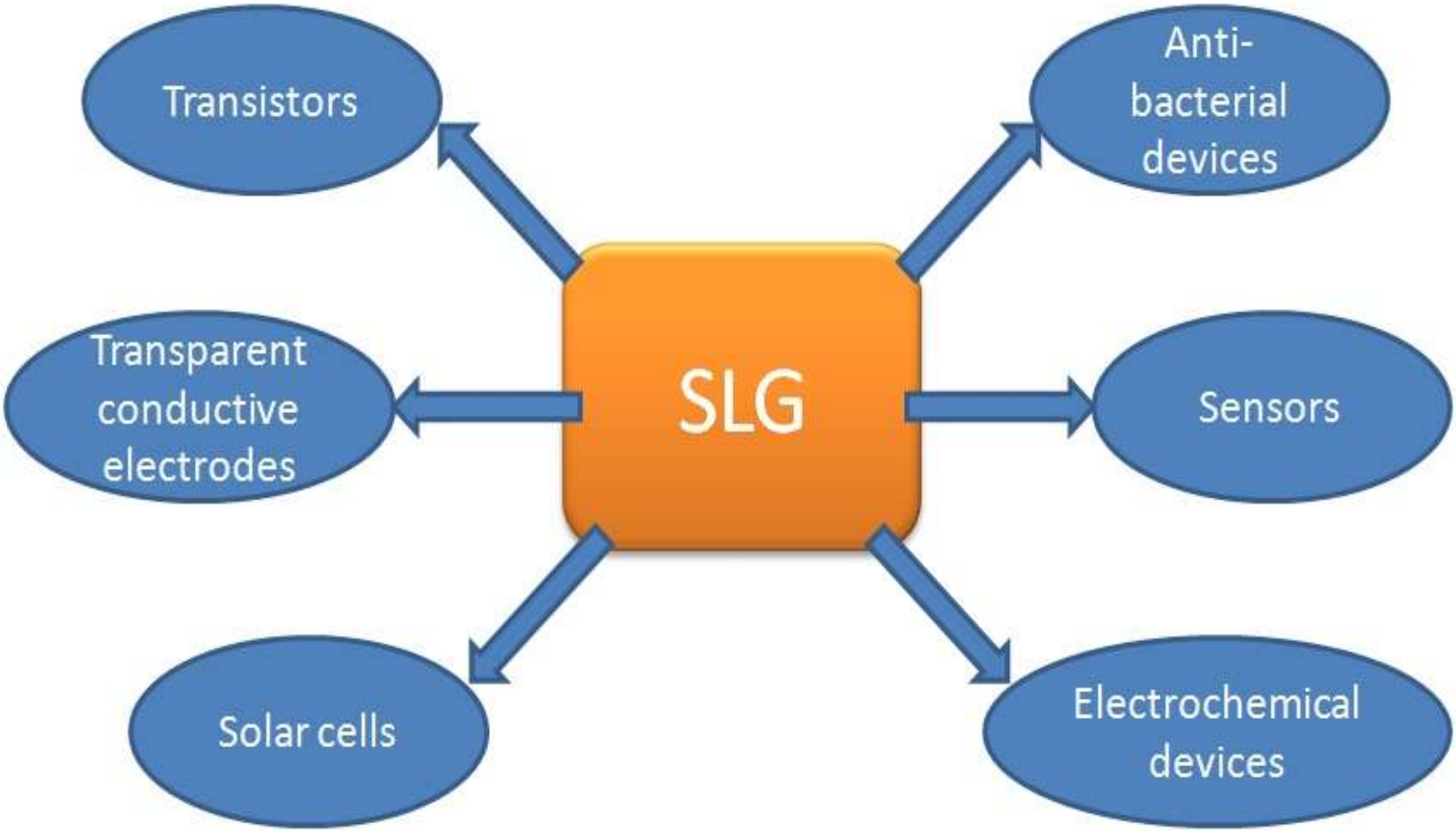
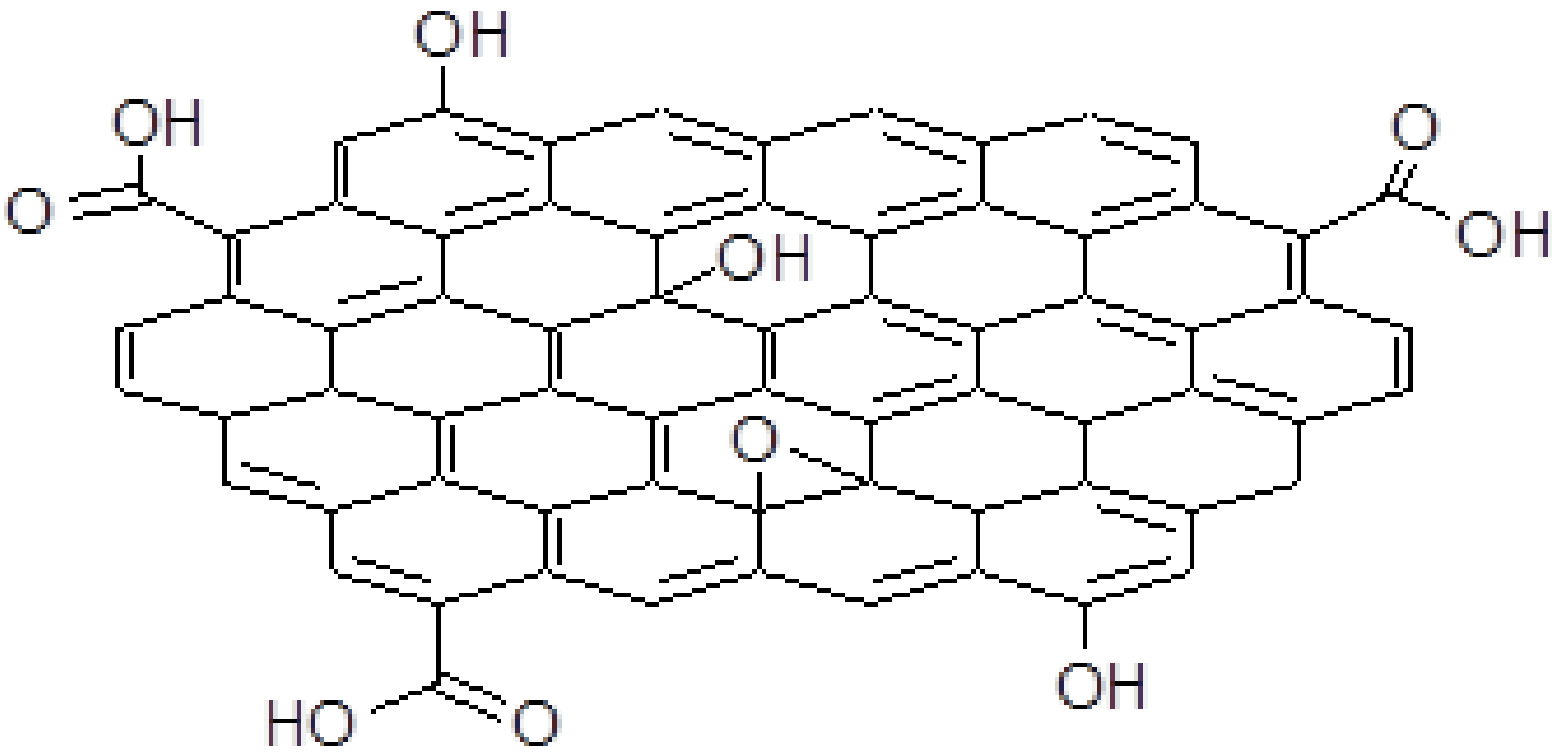
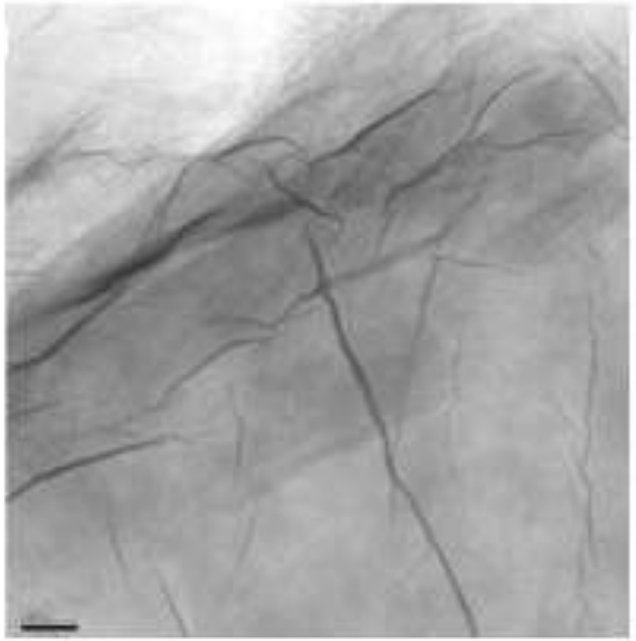
Single-layer graphene (SLG)



Single-layer graphene oxide (SLGO)



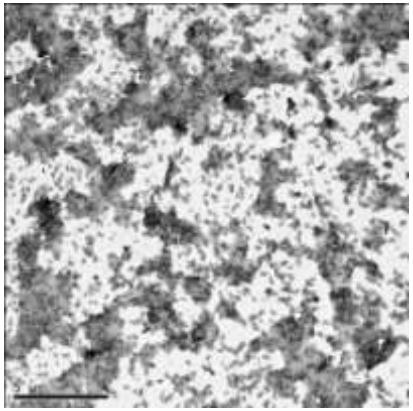
SLGO at pH7



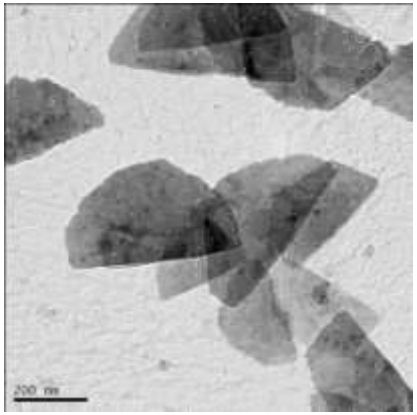
Scale bar of 1 μm

Whitby, R. L. D., A. Korobeinyk, et al. (2011). "Morphological changes and covalent reactivity assessment of single-layer graphene oxides under carboxylic group-targeted chemistry." Carbon **49**(2): 722-725.

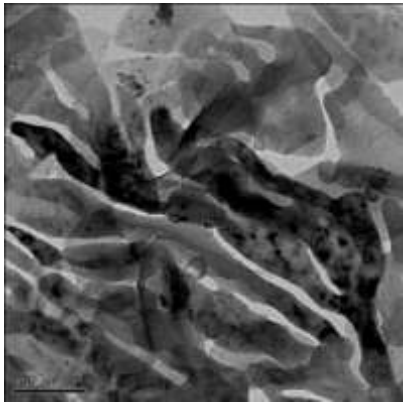
SLGO at pH3



Scale bar 5 μm



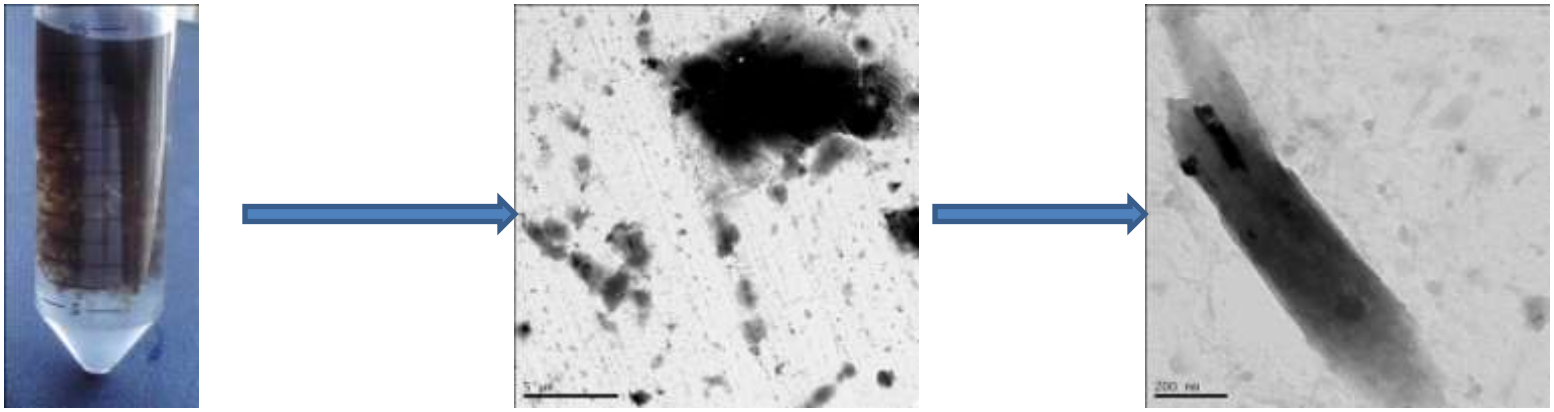
Scale bar 200 nm



Scale bar 200 nm

Whitby, R. L. D., A. Korobeinyk, et al. (2011). "pH-driven physicochemical conformational changes of single-layer graphene oxide." Chemical Communications **47**(34): 9645-9647

SLGO at pH14

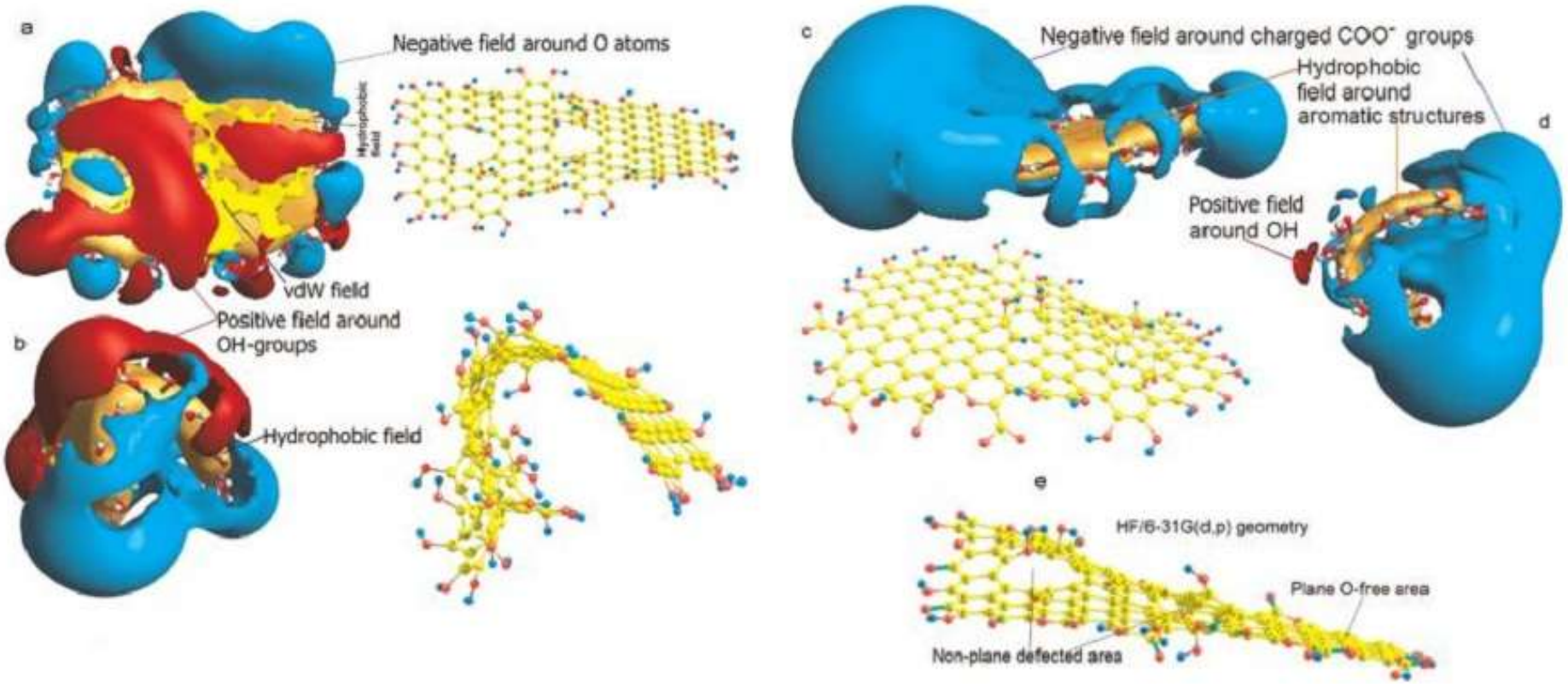


Scale bar 5 μm

Scale bar 200 nm

Whitby, R. L. D., A. Korobeinyk, et al. (2011). "pH-driven physicochemical conformational changes of single-layer graphene oxide." Chemical Communications **47**(34): 9645-9647

Field point method



Scheme of the distribution of potential fields (red= positive, blue = negative, orange= hydrophobic, yellow=van der Waals, vdW calculated using Field View 2.0.2) around a small SLGO sheet with zero total charge of (a) non bent and (b) bent sheet and negatively charged sheet (c) non bent and (d) bent; (e) *ab initio* HF/6-31G(d,p) calculation of the SLGO model showing two parts with planar O-free and non planar O-containing patches

Whitby, R. L. D., V. M. Gun'ko, et al. (2012). "Driving Forces of Conformational Changes in Single-Layer Graphene Oxide." ACS Nano **6**: 3967–3973.

Conclusions

- At low pH, numerous SLGO sheets fold a single. At high pH, each sheet undergoes extensive folding and condense against neighbouring sheets into larger macroscale agglomerates.
- The shapes of graphene sheet aggregates observed in TEM images depend on the pH at which the suspension was dried, given that conformational changes start in the aqueous medium and are enhanced during drying.
- Possible mechanism of the SLGO sheets transformation under influence of the different pH was explained through the Field point calculation method in respect to protonation or deprotonation which occurs on the oxygen containing groups of the SLGO.

Acknowledgements

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Thank you for your attention!