Editorial: 2D nanomaterials for energy research

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Following the astounding discoveries of C_{60} by Kroto, Smalley and Curl in 1985,¹ and carbon nanotubes by Iijima (1991),² Tenne *et al.* reported the first inorganic analogs in WS_2 nanoparticles back in 1992.³ As much as this new field of inorganic fullerene-like nanoparticles (IF) and inorganic nanotubes (INT) was motivated by unique scientific advances, it was also driven by the desire to exploit these nanomaterials – for example, as superior solid lubricants. Indeed, large-scale commercial application of IF- WS_2 nanoparticles as additives to numerous lubrication fluids has been recently realized. Burgeoning applications of polymer nanocomposites reinforced by adding small amounts of such nanoparticles are emerging as well. In the same vein, the discovery of graphene by Geim and Novoselov in 2004,⁴ was followed by breathtaking advances in research of two-dimensional (2D) (layered) nanosheet materials, like exfoliated MoS_2 , silicenes and so on (often named ‘beyond graphene’). While research on these nanomaterials goes back a few decades, the current research environment, encompassing both advanced experimental tools and theory, opened up a range of remarkable opportunities and stimulated frenzy research activity of such 2D nanomaterials. A clear paradigm shift to fabricating and investigating inorganic monolayer-thick and several-molecular-layers-thick films led to stunning observations. In particular, while bulk MoS_2 is an indirect bandgap semiconductor, a monolayer of MoS_2 was shown to have a direct transition and consequently exhibits strong luminescence in the visible region. Furthermore, the loss of inversion symmetry in such monolayers was shown to lift the spin degeneracy in the valence band, resulting in a new way to control the electron transport across the monolayer (valleytronics). Also, high-performance field-effect transistors with and on-off ratio of 10^8 have been realized in recent years. This last important development may lead to a paradigm shift in the future roadmap for beyond-silicon electronics.

No less important are the recent advances relevant to the field of interest of this journal. Energy research is always among the first to embrace new materials technologies, and therefore not surprisingly, soon after the discovery of graphene, many researchers focused their efforts in utilizing these new opportunities of molecular films into energy-harvesting and -storage devices. Thus cathodes for rechargeable lithium batteries with capacities exceeding 1000 mWh/g were fabricated using, for example, mixtures of different forms of nanocarbon together with nanosheets of MoS_2 (SnS_2 , metal carbides and other 2D compounds) and a polymer binder. In contrast to bulk (2D)

materials, where diffusion of the lithium ions through the galleries between the molecular layers is slow and rate-controlling, the large surface area of exfoliated MoS_2 can be easily accessed by the ions assuring fast kinetics and low overvoltage, even under high current densities. For the same reason, high-performance supercapacitors made of exfoliated MoO_3 , MoS_2 , WS_2 and metal carbide nanosheets were investigated. Also, efficient catalytic reduction of water and hydrogen production with arrays of MoS_2 and WS_2 nanosheets was reported.

The themed issue papers on ‘2D materials for energy research’ aim to showcase some of the striking advances in this area. C.N.R. Rao and co-workers⁵ studied the oxygen reduction reaction (ORR), which occurs at the cathode of a fuel cell. They fabricated electrodes from nanosheets of borocarbonitride (BC_5N)-supported iron (II) phthalocyanine and found it to be a superior non-noble electrocatalyst for the ORR. In another paper of this group,⁶ electrodes consisting of MoS_2 nanosheets and reduced graphene oxide (RGO) were fabricated. This composite was found to perform very well as supercapacitor as well as in the ORR reaction. The excellent performance of this composite was attributed to the combined effect of the high electrical conductivity of RGO and the unique surface properties of both MoS_2 and RGO. Višić⁷ reviewed the synthesis of monolayer-thick MoS_2 nanosheets and some of their outstanding electrical and optical properties. Sedova *et al.*⁸ reported on the excellent solid lubrication properties of rhenium doped IF- MoS_2 nanoparticles in relation to bio-medical applications. Given the bio-compatibility of such nanoparticles, this technology may have substantial impact on such medical technologies as urology, angioplasty and so on. A multiscale first principle (molecular dynamics) approach for the study of the thermal properties of polymer composites impregnated with carbon nanostructures was reported by Unnikrishnan.⁹ Atomistic simulation was used to study the interfacial thermal resistance between the carbon nanotubes and low-density polyethylene. The model allows predicting the thermal properties of such nanocomposites as a function of the nanotubes’ radius, length and their packing fraction.

In conclusion, these themed issue papers dedicated to 2D nanomaterials presented some of the frontiers in this emerging field, which is likely to have major impact on energy research and development for years to come.

REFERENCES

1. Kroto, H. W.; Heath, J. R.; O'Brien, S. C.; Curl, R. F.; Smalley, R. E. C₆₀: Buckminsterfullerene. *Nature* **1985**, *318*, 162–163.
2. Iijima, S. Helical microtubules of graphitic carbon. *Nature* **1991**, *354*, 56–58.
3. Tenne, R.; Margulis, L.; Genut, M.; Hodes, G. Polyhedral and cylindrical structures of tungsten disulphide. *Nature* **1992**, *360*, 444–446.
4. Novoselov, K. S.; Geim, A. K.; Morozov, S. V.; Jiang, D.; Zhang, Y.; Dubonos, S. V.; Grigorieva, I. V.; Firsov, A. A. Electric field effect in atomically thin carbon films. *Science* **2004**, *306*, 666–669.
5. Moses, K.; Pramoda, K.; Rao, C. N. N. Use of a borocarbonitride–iron phthalocyanine composite in ORR. *Nanomaterials and Energy* **2015**, *4*, 3–8.
6. Gopalakrishnan, K.; Pramoda, K.; Maitra, U.; Mahima, U.; Shah, M. A.; Rao, C. N. R. Performance of MoS₂-reduced graphene oxide nanocomposites in supercapacitors and in oxygen reduction reaction. *Nanomaterials and Energy* **2015**, *4*, 9–17.
7. Višić, B. Silver nanoparticle synthesis mediated by carboxylated cellulose nanocrystals. *Nanomaterials and Energy* **2015**, *4*, 18–29.
8. Sedova, A.; Ron, R.; Goldbart, O.; Elianov, O.; Yadgarov, L.; Kampf, N.; Rosentsveig, R.; Shumalinsky, D.; Lobik, L.; Shay, B.; Moshonov, J.; Wagner, H. D.; Tenne, R. Re-doped fullerene-like MoS₂ nanoparticles in relationship with soft lubrication. *Nanomaterials and Energy* **2015**, *4*, 30–38.
9. Unnikrishnan, V. U. Interfacial thermal properties and size-effect in thermo-mechanical characterisation of nanocomposites. *Nanomaterials and Energy* **2015**, *4*, 39–44.