Adsorption and Separation of Carbon-Monoxide on Metal-decorated Graphene Oxide

Lu Wang[1], Jijun Zhao[1]*, Yiyang Sun[2], Shengbai Zhang[2]

[1]Key Laboratory of Materials Modification by Laser, Ion and Electron Beams (Dalian University of Technology), Ministry of Education, Dalian 116024, P. R. China
[2]Department of Physics, Applied Physics, and Astronomy, Rensselaer Polytechnic Institute, Troy, New York 12180, USA
*Corresponding author: zhaojj@dlut.edu.cn

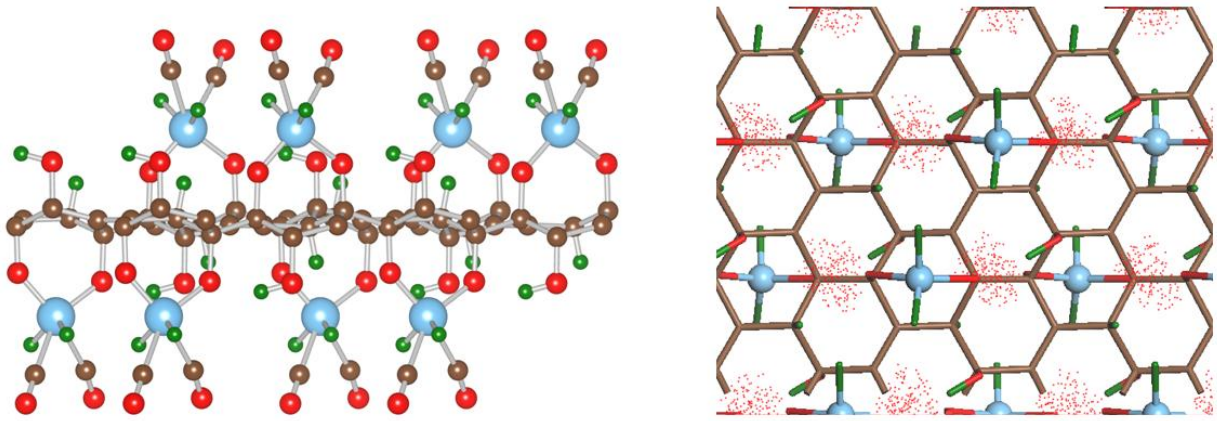
As the superstar in current nanoscience, graphene and related nanomaterials have attracted continuous interests in the past years, and have many applications in a variety of fields. Among these graphene related nanomaterials, graphene oxide (GO) has attracted resurgent attentions in recent years, though graphite oxide has been synthesized for more than 150 years. In our previous works, we have systematically investigated the structural stability of GO phases [1] and predicted that transition metal (e.g., Ti) anchored on GO can absorb molecular hydrogen at the room temperature avoiding metal clustering [2]. Here we will explore the potential applications of GO in the environmental field.

Release of toxic and exhaust gases into environment is a growing national concern and effective capture of these gases is an urgent issue to the environment protection. Finding the ideal sorbents for gas capture and separation is of great importance, and previous efforts have been focused on zeolites and metal-organic frameworks (MOF) materials due to their thermal stability, structural porosity, and high adsorption capacity. Separation and removal carbon monoxide (CO) from natural gas is one of the industrially significant separation processes and is an important issue in fuel cell technology. As the gas sorbents, GO has light mass with large surface area, very low cost and can be easily chemical modified. Here we will propose metal-decorated GO as an ideal sorbent for CO adsorption and separation from the natural gas (e.g., N_2) or the other gas mixtures (e.g., CH_4). The adsorption capacity and selectivity of different toxic and exhaust gases on the metal-decorated GO surface has been comprehensively studied using first-principles calculations and Grand Canonical Monte Carlo simulations. In addition to understand the binding strength and electronic effects of the gas adsorbed on the metal-decorated GO substrate, we further explore the possibility of selection/separation of gas mixture. Moreover, different decorated metals exhibit different adsorption capacities for gases.

References

[1] L. Wang, Y. Y. Sun, K. Lee, D. West, Z. F. Chen, J. J. Zhao, and S. B. Zhang, Phys. Rev. B **82** (2010) 161406.
[2] L. Wang, K. Lee, Y. Y. Sun, M. Lucking, Z. F. Chen, J. J. Zhao, and S. B. Zhang, ACS Nano, **3** (2009) 2995.

Figures



(a) Optimized structures of Ti-decorated GO with fully loaded CO adsorption from first-principles calculations, brown balls denote carbon atoms, red balls for oxygen atoms, green balls for hydrogen atoms and light blue for titanium atoms; (b) Density distributions for CO molecules on the Ti-decorated GO at the condition of 298 K and 10 Bar using the Grand Canonical Monte Carlo simulations, and the red points are the centers-of-mass of the adsorbed CO molecules.