

METHANE AND HYDROGEN ADSORPTION ON GRAPHENE

J. Vekeman¹, I. Garcia Cuesta¹, N. Faginas Lago², J. Sánchez Marin¹, A. M. Sánchez de Merás¹

¹ *Instituto de Ciencia Molecular, Universitat de València, Cat. Jose Beltran Martinez 2, 46980 Paterna, Spain.*

² *Dipartimento di chimica, biologia e biotecnologie, università di Perugia, Via Elce di Sotto 8, 06123 Perugia, Italy.*

Graphene is widely investigated for its ability to adsorb small molecules through van der Waals interactions, possibly leading to new ways of natural gas storage. Given the environmental issues of our time, hopes are that graphene could play an important role in capture and separation of greenhouse gases from gas mixtures. From those greenhouse gases methane is one of the most abundant and most active gases around. Diminishing its emissions is therefore of utmost importance. One way to lower the emissions is by filtering CH₄ from gas mixtures before releasing the mixture into the atmosphere. The aforementioned qualities of graphene make the material a good candidate for the proposed tactics. Furthermore, graphene has shown promise as a material for energy storage. The adsorption and controlled release of gases like methane and hydrogen may lead to efficient clean energy technologies.

In this work interaction energies for graphene-X and X-X (X being CH₄ or H₂) were calculated using the DFT-method with the B97D functional and a TZV2P basis set. The basis set superposition error was minimized by means of the counter-poise correction. The results were fitted to Improved Lennard-Jones[1] type potentials in order to get a set of parameters describing the dispersion interactions of interest. Aside from this, the parameters were also calculated from correlation formulae[2] at DFT, CC2, CC3 and CCSD level. The influence of inclusion of the Coulombic sum has also been investigated. This way we obtained numbers from different levels of theory to ensure parameters describing an accurate potential energy. We aim at producing potentials that are on one hand very accurate, but on the other easily compatible with molecular dynamics. The resulting potentials were compared with energies from highly correlated ab initio methods in order to assure accuracy. The created force fields are applied in molecular dynamics and grand canonical Monte Carlo dynamics to calculate adsorption isotherms, diffusion coefficients and other relevant characteristics.

Acknowledgments: This work has the support of the European joint doctorate program on theoretical chemistry and computational modelling within the frame of the innovative training networks of the Marie Skłodowska-Curie actions.

References

- [1] F. Pirani, S. Brizi, L. F. Roncaratti, P. Casavecchia, D. Cappalletti, F. Vecchiocattivi, *Phys. Chem. Chem. Phys.*, **10**, 5489 (2008).
- [2] R. Cambi, D. Cappalletti, G. Liuti, F. Pirani, *J. Chem. Phys.*, **95**, 1852 (1991).