Multi-scale studies of gas-substrate interactions: Benchmarks and applications

M. Hochlaf

Université Gustave Eiffel, COSYS/LISIS, 5 Bd Descartes 77454, Champs sur Marne, France.
email: hochlaf@univ-mlv.fr

Using first principles approaches, we characterized the bimolecular interactions between medium-sized molecules (imidazole, triazole, …) and gases (*e.g.* CO_2, H_2O). The medium-sized molecule is either isolated, attached to a metallic cluster or a metallic surface. For this purpose, the minimum energy geometries corresponding to these systems have been searched and optimized using various *ab initio* and DFT methods. Accurate energetics are derived using the newly tested explicitly correlated coupled cluster approaches. We also established the good performance of M05-2X (+D3) and PBE0 (+D3) DFTs for the accurate description of these systems and therefore that of the larger macromolecular structures. Moreover, we found that the bimolecular complex formation process can follow energetically favored multi-channel. Hence, we mapped their interaction potentials along the intermonomer coordinates. Our calculations show that long-range interactions between these medium-sized molecules and gases are strongly dependent on the electronic correlation. *In fine*, we establish the universality of the type of the interactions governing the clustering of gases with these medium-sized molecules either isolated, attached to gold cluster, gold surface or within the ZIFs. For illustration, diverse examples will be presented [1-11].

Acknowledgments

The authors extend their appreciation to the International Scientific Partnership Program (ISPP) at King Saud University for funding this research work through ISPP# 0045. We thank a Marie Curie International Research Staff Exchange Scheme Fellowship within the 7th European Community Framework Programme under Grant No. IRSES-GA-2012- 31754 and COST ACTION CM1405 MOLIM.

References

1. M. Prakash, K. Mathivon, D. M. Benoit, G. Chambaud and M. Hochlaf. Phys. Chem. Chem. Phys. **16**, 12503 (2014).
2. M. Prakash, G. Chambaud, M. Mogren Al-Mogren and M. Hochlaf. J. Mol. Mod. **20**, 2534 (2014).
3. S. Dalbouha, M. Prakash, V. Timón, N. Komiha, M. Hochlaf and M. L. Senent. Theo. Chem. Accounts **134**, 63 (2015).
4. V. Timon, M. L. Senent and M. Hochlaf. Microporous and Mesoporous Materials **218**, 33 (2015).
5. K. Boussouf, R. Boulmene, M. Prakash, N. Komiha, M. Taleb, M. Mogren Al-Mogren and M. Hochlaf. Phys. Chem. Chem. Phys. **17**, 14417 (2015).
6. K. Boussouf, T. Khairat, M. Prakash, N. Komiha, G. Chambaud and M. Hochlaf. J. Phys. Chem. A **119**, 11928 (2015).
7. R. Boulmene, K. Boussouf, M. Prakash, N. Komiha, M. M. Al-Mogren and M. Hochlaf. ChemPhysChem **17**, 994 (2016).
8. R. Boulmène, M. Prakash and M. Hochlaf. Phys. Chem. Chem. Phys. **18**, 29709 (2016).
9. B. C. M. Arputham Ashwin, A. H. Arun Baby, M. Prakash, M. Hochlaf and P. Muthu Mareeswaran. J. Phys. Org. Chem. **31**, e3788 (2018).
10. R. Dahmani, S. Ben Yaghlane, S. Boughdiri, M. Mogren Al-Mogren, M. Prakash and M. Hochlaf. Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy **193**, 375 (2018).
11. R. Dahmani, S. Grubišić, S. Ben Yaghlane, S. Boughdiri and M. Hochlaf. J. Phys. Chem. A 123, 5555 (2019).