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Chemical Physics Letters 392 (2004) 567
CHEMICAL PHYSICS LETTERS
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Corrigendum

Corrigendum to: 'Interaction of functionalized benzene molecules with carbon nanopores' [Chem. Phys. Lett. 389 (2004) 96] ☆

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Received 3 May 2004
Available online 19 June 2004

Calculation of the adhesion energies of weakly bound systems is a challenging endeavor to undertake. It is with regret that we did not include in our Letter a discussion of the ongoing dialogue in the literature of the strengths and weaknesses of our selected technique's ability to describe such systems. Density functional theory (DFT) using the generalized gradient approximation of Perdew and Wang (GGA-PW91) [1,2] to represent the contribution of exchange and correlation energy to the total energy, the technique used in our Letter, has been shown to give reasonable energies for systems dominated by dispersion interactions [3]. Møller–Plesset second-order perturbation theory [4,5] and coupled cluster calculations with singles and doubles substitutions and non-iterative triples [6] techniques are preferred for very a accurate evaluation of adsorption energies in these systems. However, the relatively large system sizes in our calculations (as large as 165 atoms) make these techniques too computationally intensive to be used. DFT with the GGA-PW91 approximation underestimates bond energies and predicts slightly larger bonding distances compared to these more accurate methods. However, both the trends presented and the overall finding of poor selectivity for substituted benzene molecular adsorption to nanoporous carbon materials should be qualitatively accurate.

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☆ DOI of original article 10.1016/j.cplett.2004.03.073.
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doi:10.1016/j.cplett.2004.05.110