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Confinement effects on excitation energies and regioselectivity as probed by the Fukui function and the molecular electrostatic potential ALEX BORGOO, Vrije Universiteit Brussel, DAVID TOZER, Durham University, PAUL GEERLINGS, FRANK DE PROFT, Vrije Universiteit Brussel — When a molecule is placed as a guest inside a zeolite pore, its electronic structure will be altered, among others by the effect of the so-called "confinement". It has been established that the compression of the molecular orbitals influences a system's reactivity. In this work we use a simple potential barrier method to quantify the importance of confinement effects on chemical reactivity. In the first part, excitation energies and molecular orbital energy gaps are evaluated for molecules placed in cavities of different sizes. Our results for ethylene and formaldehyde reveal an increase in excitation energy and the gap between the occupied and the unoccupied levels. In the case of the larger molecules naphthalene and anthracene, the HOMO-LUMO gap shows very little sensitivity to the confinement. To investigate the role of confinement effects on local aspects of chemical reactivity and on regioselectivity, we evaluated its effect on the Fukui function and the molecular electrostatic potential, reactivity indices that are central in the description of orbital and charge controlled reactions. The results indicate that confinement can influence the regioselectivity and that the reactivity of anions is expected to change, due to the artificial binding of the exess electron.

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