

Chemistry in a Field

by

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Measuring the bonding energies or scanning the potential energy surface (PES) of the charged molecular systems in the presence of external electric field (EEF) requires a careful evaluation of the origin-dependency of the energy of the system and references. Scanning the PES for charged or purely ionic systems for obtaining the intrinsic energy barriers needs careful analysis of the electric work applied on ions by the EEF. Meaning of the binding energy in the presence of EEF is different from that in the absence of electric field as the binding energy is an anisotropic characteristic which depends on the orientation of molecules with respect to the EEF. In this contribution we discuss various aspects of PES in the EEF and the concept of binding energy in the presence of EEF. In addition, we demonstrate that the anion- π bonding properties can be modulated by applying the uniform EEF, which has a more pronounced effect on the larger, more polarizable π -systems. We predict that understanding the phenomenon introduced in the present account has an enormous potential, for example, for separating charged species on the surface of polarizable two-dimensional materials such as graphene or the surface of carbon nanotubes, in desalination of water.

