

# Metal–organic molecular interfaces: Options for induced structure manipulation

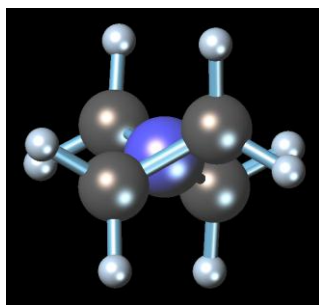
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Interfaces between metal atoms and organic molecules are key units of metal–organic frameworks, contacts between metal electrodes and molecular “wires”, catalysis–related species. One class of such interfaces is represented by sandwich–type complexes with the molecules on both sides of the atoms. Most of previously studied such systems involve transition metals, while main–group light metals may introduce features related to closer proximity of the molecules combined with their favoured orientation [1].

Presented are results of ab initio calculations for a series of complexes of light–metal atoms sandwiched between small unsaturated hydrocarbons [1, 2]. Evolution of the system structure and stability with the metal atom, as well as with ionization and electron attachment, is systematically studied. Interesting features include non–additive stabilization on adding molecule to the half–sandwich precursor, unusual geometries in some cases, and reversible charge–state dependent geometry variations. Such properties apparently suggest potential applications of the above species as stable intermolecular junctions and units with charge–controlled shapes (switches) in molecular devices and/or machines.

Also of interest is the metal–atom induced fusion of the sandwiching molecules, leading to another isomer of the system. Different metals are predicted to favour different isomers, with such a process producing higher–energy species in some cases. Furthermore, the relative stabilities of the two isomers depend on the charge state, offering further options for structure manipulation.



[1] Naumkin, F. Y., *Chem. Phys. Lett.* 499:203, 2010.

[2] Naumkin, F. Y., submitted (2013).