

The silane-methane dimer revisited: more than a dispersion-bound system?

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Supporting Information

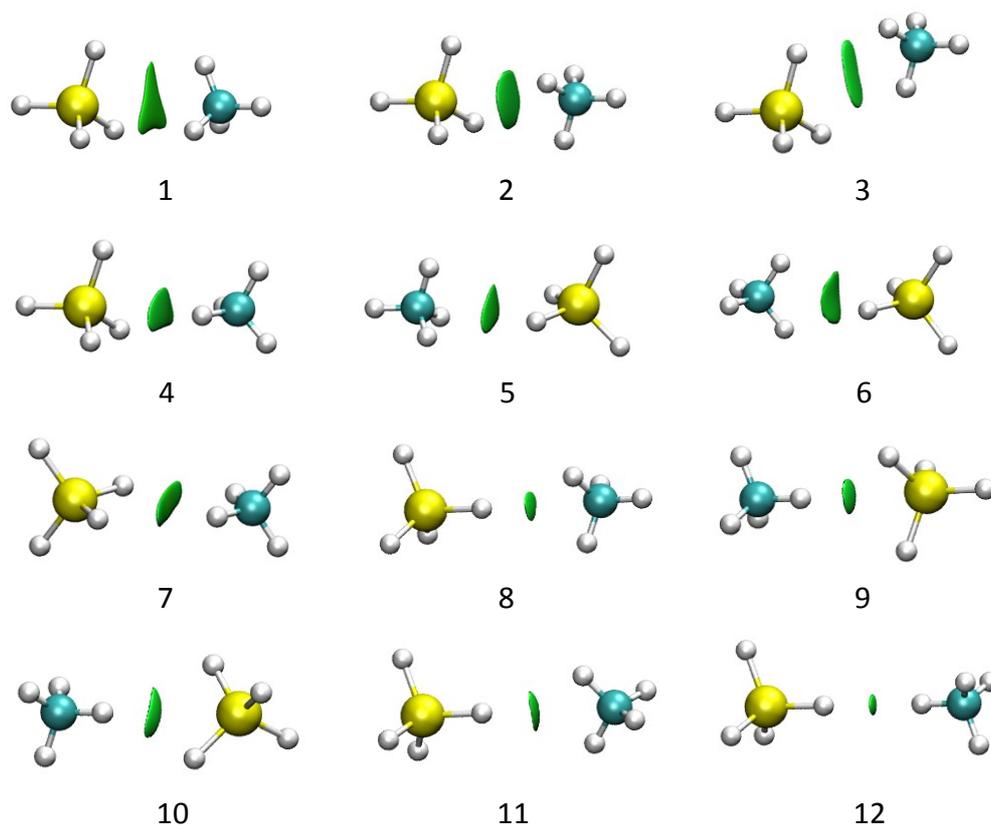


Figure S1. NCI plots for silane-methane dimers with interaction topologies **1** – **12**.

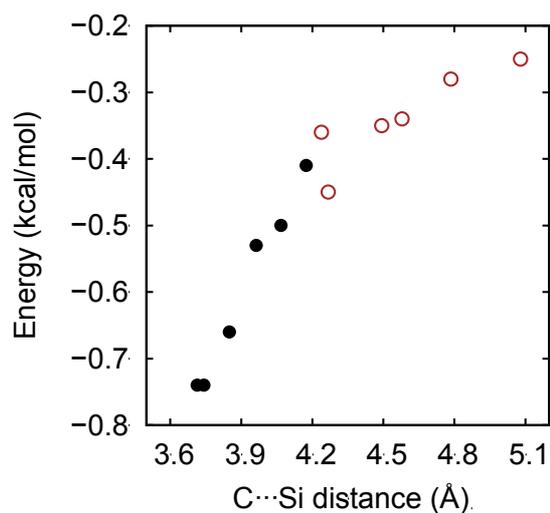


Figure S2. Binding energy as a function of the C...Si intermolecular distances in silane-methane dimers with topologies **1** – **12**. The black points represent interaction geometries in which the C...Si contacts are topologically favored (**1** – **6**).

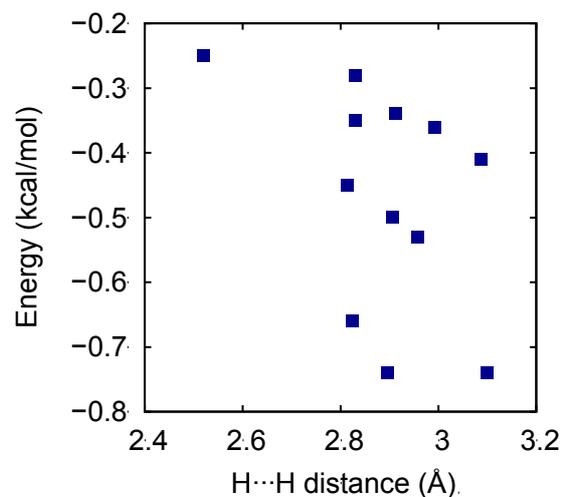


Figure S3. Binding energy as a function of the shortest intermolecular H...H distance in methane-silane dimer with interaction topologies **1 – 12**.

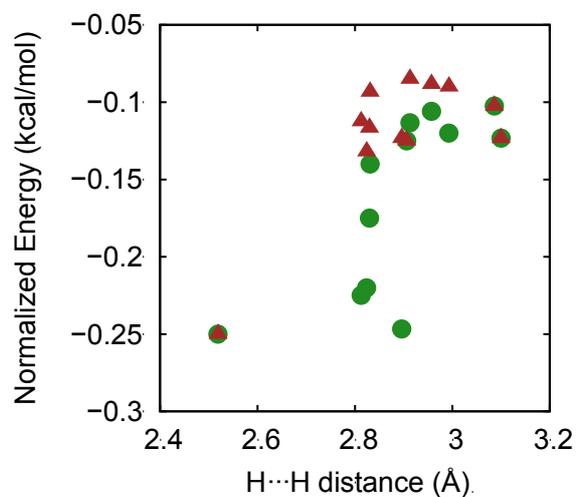


Figure S4. Normalized binding energy (per number of H atoms involved in the interaction, in red; and per number of H...H contacts shorter than 3.3 Å, in green) as a function of the shortest intermolecular H...H distance in methane-silane dimers with interaction topologies **1 – 12**.

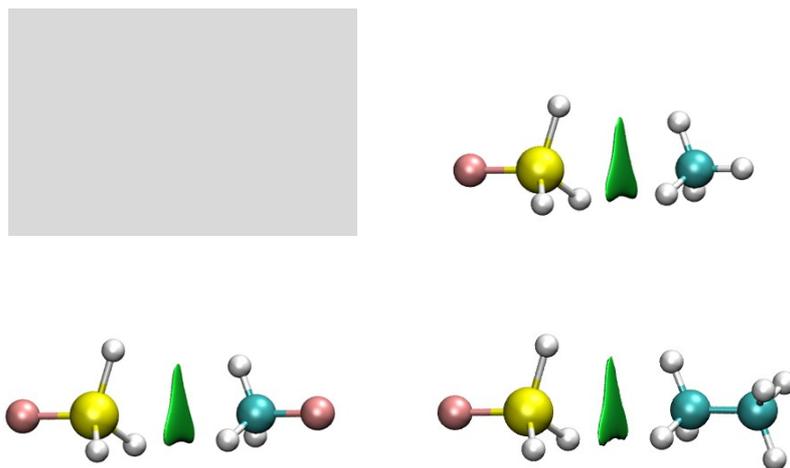


Figure S5. NCI plots for the silane-methane dimer and several of its derivatives with interaction topology **1** (Colour code: yellow = Si, blue = C, pink = F, white = H).

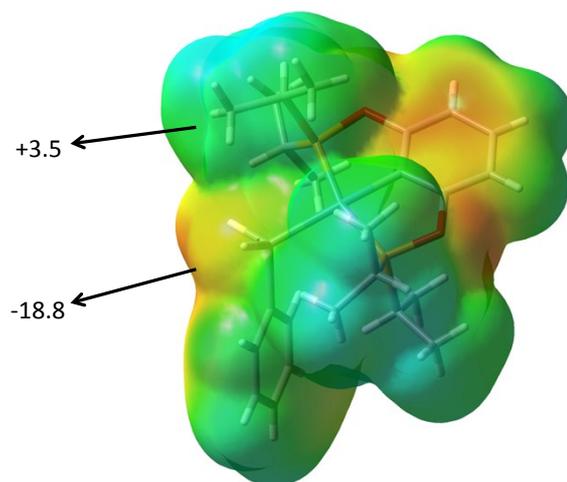


Figure S6. MEP map of the dimer found in the crystal structure of the CSD refcode zuzhuz. V_s values are given in kcal mol⁻¹.