In depth description of forces that drive atoms to binding or molecules to aggregation is very crucial from both theoretical and experimental points of view. Such knowledge allows not only for understanding structure, reactivity and various phenomena, but also for rational design of other systems exhibiting desired properties. Very important are non-covalent interactions which are relatively weak (binding energies are up to several kcal/mol), however, they are responsible for plethora of events including for example molecular self-assembling, electron transfers or drug transportation. Hompolar dihydrogen interactions XH•••HX (X – various atoms of the periodic table), abbreviated as HOMO-DHI, are yet unexplored in comparison with other non-covalent interactions. Furthermore, they are considered by the majority of scientists as the source of steric repulsion. As example one can provide the steric repulsion which occurs when bulky molecular fragments are close to each other – it is well known from organic chemistry text books, that the ground state staggered ethane is more stable than the corresponding eclipsed isomer, or cis-2-butene, where the methyl units are in close CH•••HC contact, is less stable than the parent trans-2-butene. It is interpreted as evidence of repulsive nature of intramolecular CH•••HC interactions. The applicant has recently demonstrated, based on quantum chemical calculations, that the well-established concept based on the repulsive nature of intramolecular CH•••HC interactions in cis-2-butene fails to correctly describe the origin of lower stability of cis-2-butene vs trans-2-butene. Accordingly, the nature of DHI is scheduled to be systematically revisited by using a multidisciplinary “bottom-top” approach – starting with single molecules (e.g. an unsolved riddle on the origin of relative stability of hydrocarbons: branched vs linear), and then, going through larger hydrogen storage systems (e.g. hydrides, boranes), to end up with studying DHI in macromolecules (e.g. host-guest systems, protein chains). The expected results will not only provide novel systematic knowledge on the nature of XH•••HX interactions (and accordingly, an entirely unique rationale of the molecular stability), but also shed light on a mechanism of hydrogen release, which, in turn, shall help in more rational design of useful hydrogen storage systems. The crucial theoretical outcomes will be verified in collaboration with experimental groups. The obtained fundamental knowledge shall be important for developing cleaner, non-hydrocarbon based, energy sources. Additionally, our results can lead to discovery of entirely new avenues in terms of protein folding, a mechanism of interstellar dihydrogen formation, or open a new field on supramolecular assemblies driven by homopolar DHI.