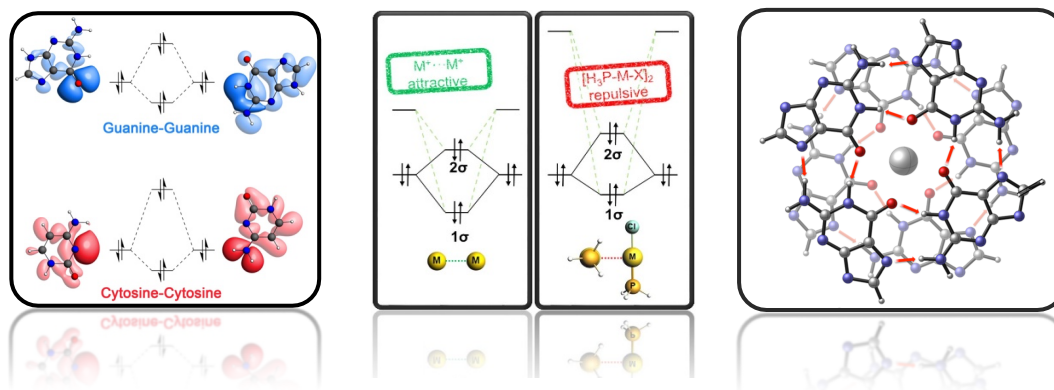


# Explaining Chemistry with repulsive Frontier Orbitals

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The importance of the Pauli (steric) repulsion in the different types of chemical interactions in supramolecular chemistry will be revealed. With the utilization of Kohn-Sham molecular orbital theory and the energy decomposition analysis, three computational studies will be presented to highlight the manifestation of the Pauli repulsive interactions: i) hydrogen bonding in the mismatched DNA base pairs CC and GG (C=cytosine, G=guanine)<sup>1</sup> and NMR <sup>1</sup>H-shielding constants,<sup>2</sup> ii) metallophilic interaction in atomic dimers ( $M^+ \cdots M^+$ ) and molecular perpendicular  $[H_3P-M-X]_2$  (where M = Cu, Ag, Au and X = F, Cl, Br, I),<sup>3</sup> iii) cation selectivity at the internal cavity site of guanine quadruplexes in telomeric DNA.<sup>4,5</sup> Understanding of the bonding mechanism of these sort of interactions will enable chemists to tune, predict and manufacture new materials in a more efficient way.



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