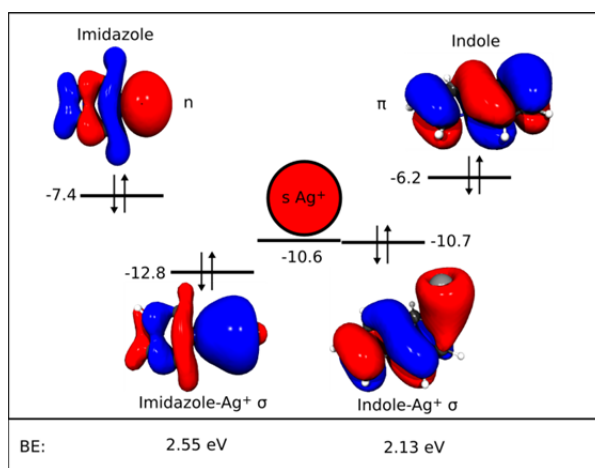


Binding motifs of silver in Prion octarepeat model peptides: a joint ion mobility, IR and UV spectroscopies, and theoretical approach.

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Scheme S1: Binding energetics of Imidazole-Ag⁺ and Indole-Ag⁺ fragments. Top: Kohn-Sham molecular orbital diagram of the involved Indole and Imidazole frontier orbitals, schematic representation of the empty silver s orbital and the resulting binding Imidazole-Ag⁺ and Indole-Ag⁺ sigma orbitals (energies in eV; n: nitrogen centered nonbonding orbital of imidazole; π: highest π orbital on indole; antibonding orbitals are not shown). Bottom: Binding energy of Ag⁺ to Imidazole and Indole.