Supplementary Material

Optical properties of AgAu clusters: effect of chemical configuration along a rearrangement pathway

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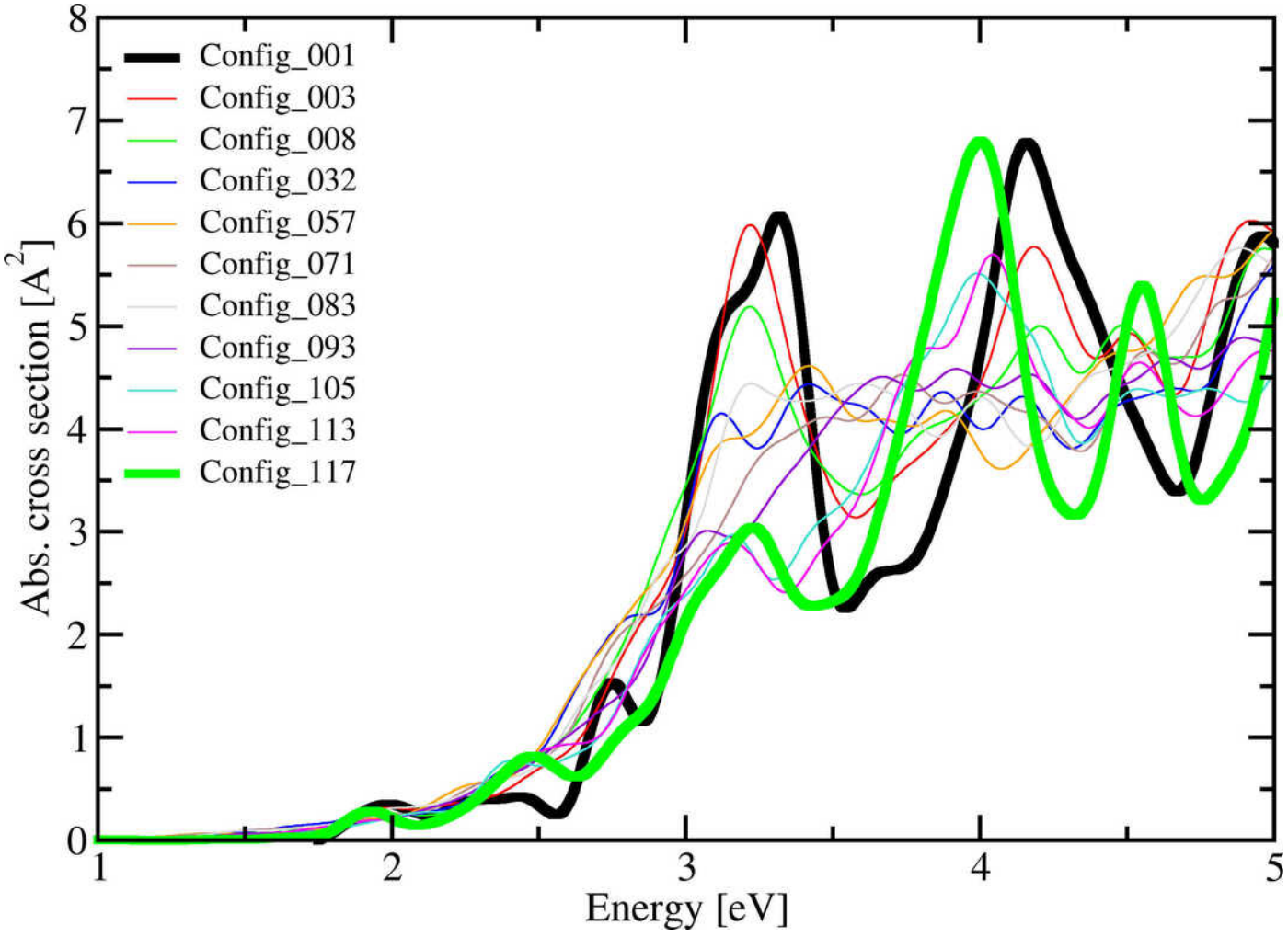
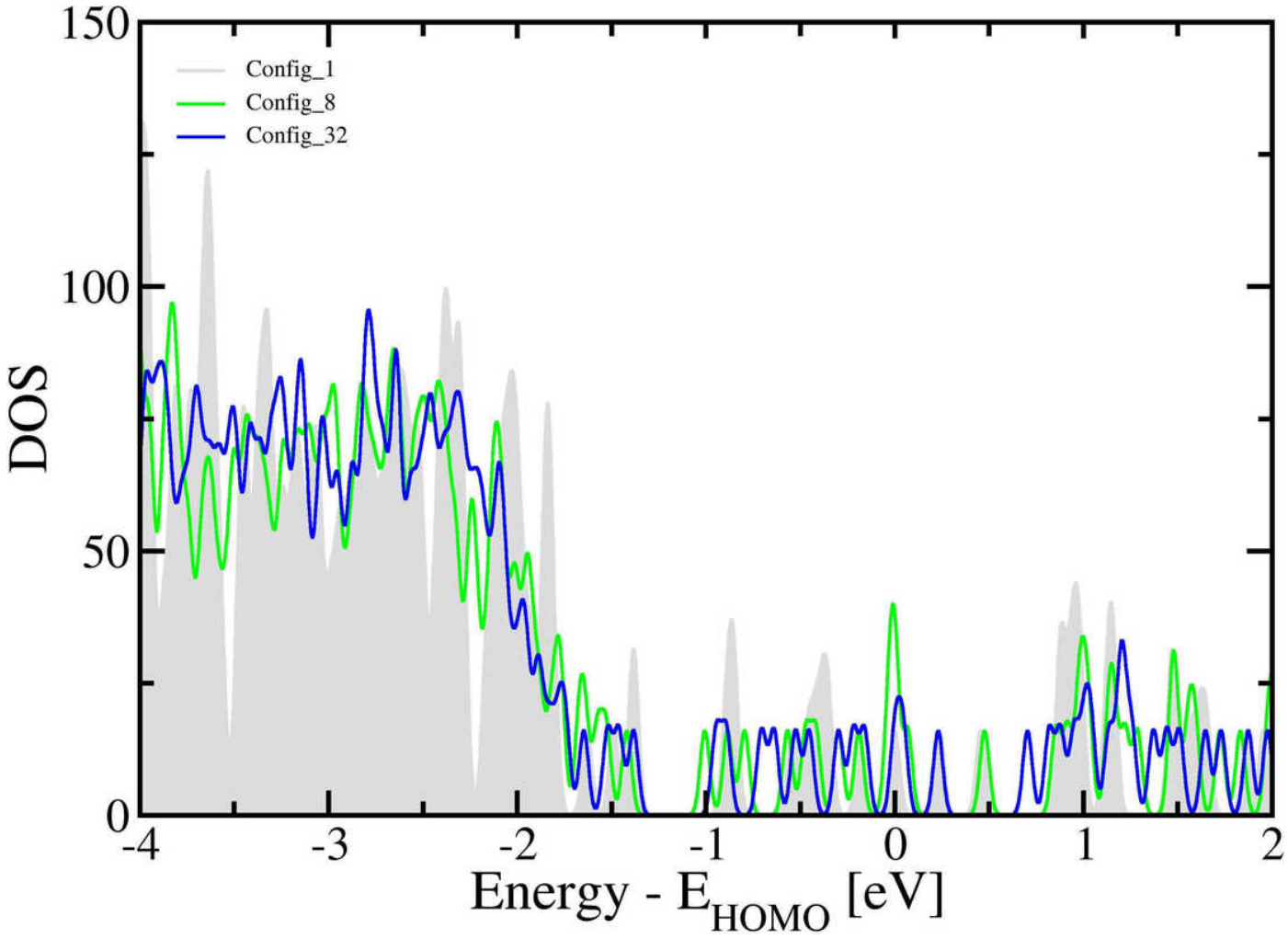
Spectra along rearrangement trajectory, $Ag_{27}Au_{28}$



Config_001 = Au_{core}, Config_001 = "intermediate", Config_117 = Ag_{core}

(cf. Figure 2 of main article)

Total DOS along rearrangement trajectory, $Ag_{27}Au_{28}$



Config_001 = Au_{core}, Config_001 = "intermediate", Config_117 = Ag_{core}

(cf. Figure 3 of main article)

Spectra of pure and core-shell AgAu 55-atom clusters

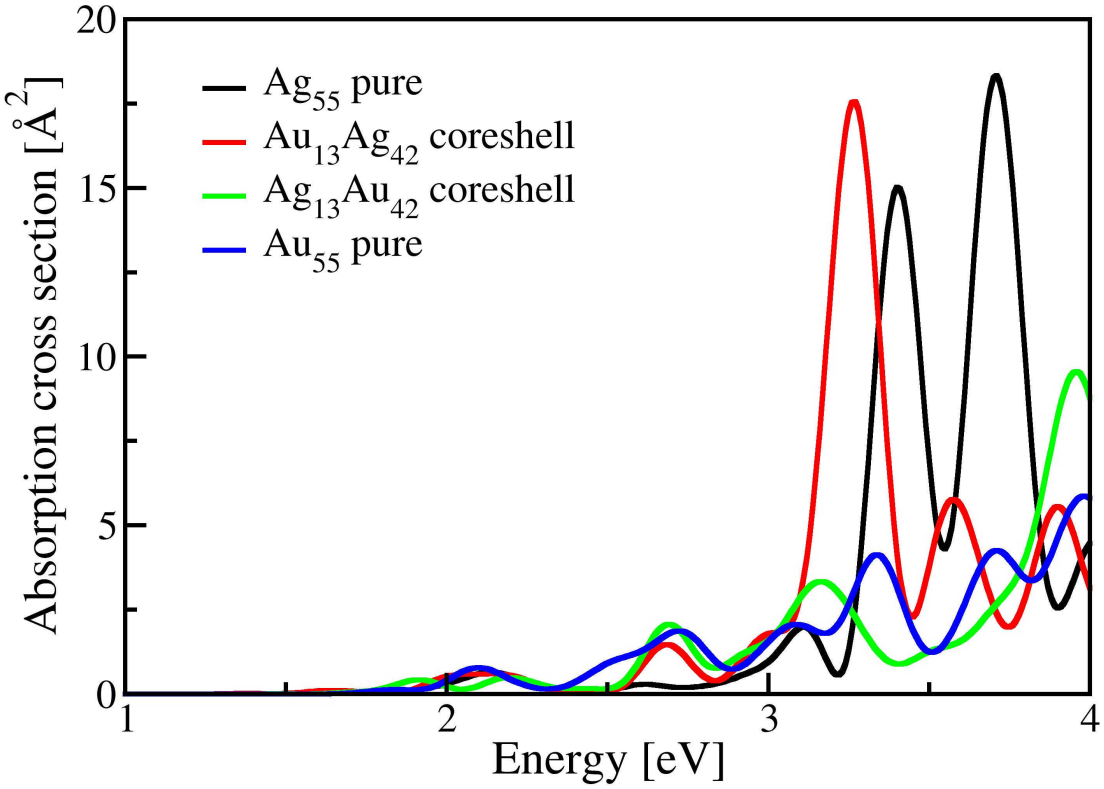


Figure: Calculated spectra of the pure 55-atom Ag and Au clusters and the two possible perfect core-shell structures with Ag and Au outer atoms, corresponding to the two compositions 13/42 and 42/13. The spectra are equivalent to those in Lopez-Lozano *et al.*, J. Phys. Chem. C, **117**, 3062–3068 (2013).

PDOS of pure and core-shell AgAu 55-atom clusters

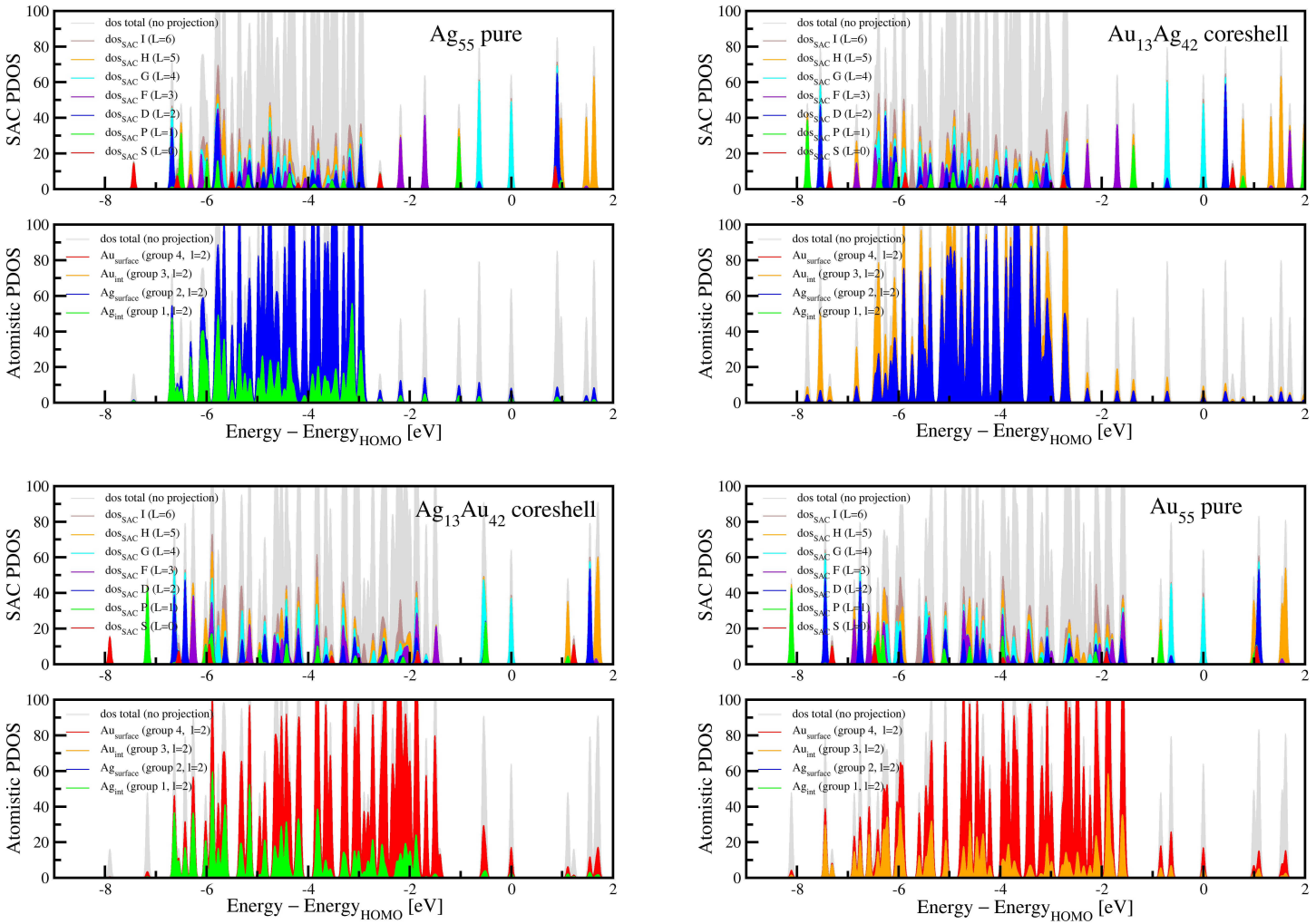


Figure: Projected densities of states of the pure 55-atom Ag and Au clusters and the two possible perfect core-shell structures with Ag and Au outer atoms, corresponding to the two compositions 13/42 and 42/13. In each case, the SAC projection (upper panels) along with the d contributions of the atomistic PDOS (lower panels) are shown. The latter are resolved into groups corresponding to the interior and surface atoms of each element.