

Supporting Information

Biopolymer-based composite hydrogels embedding small silver nanoparticles for advanced antimicrobial applications. Experimental and theoretical insights

Moises A. Rojas ¹, John Amalraj ^{2,*}, and Leonardo S. Santos ^{1,*}

¹ Laboratory of Asymmetric Synthesis, Instituto de Química de Recursos Naturales, Universidad de Talca, Talca, Chile

² Laboratory of Materials Science, Instituto de Química de Recursos Naturales, Universidad de Talca, Talca, Chile

* Correspondence: jamalraj@utalca.cl (J.A) and lssantos@utalca.cl (L.S.S)

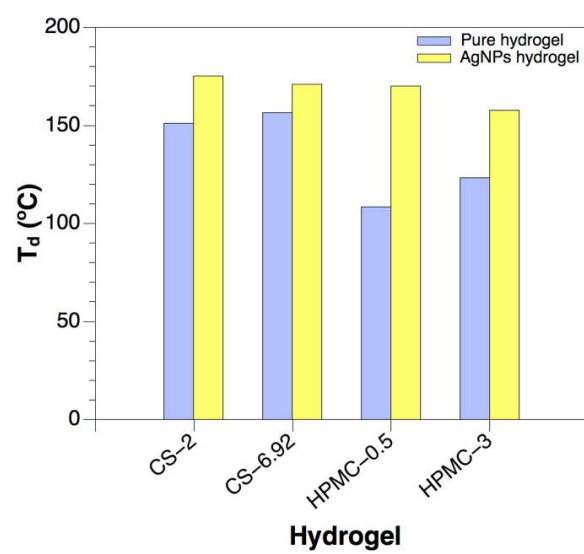


Figure S1. Denaturation temperatures (T_d , °C) for the pure CS and HPMC hydrogels and their silver nanocomposites were measured using DSC.

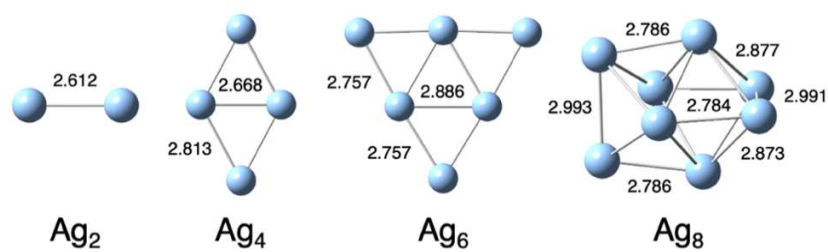


Figure S2. Optimized structures of silver nanoclusters (Ag_n) at the B3LYP/LANL2DZ level of theory, with geometries of one ($n = 2$), two ($n = 4, 6$) and three ($n = 8$) dimension. Bond lengths in Å.

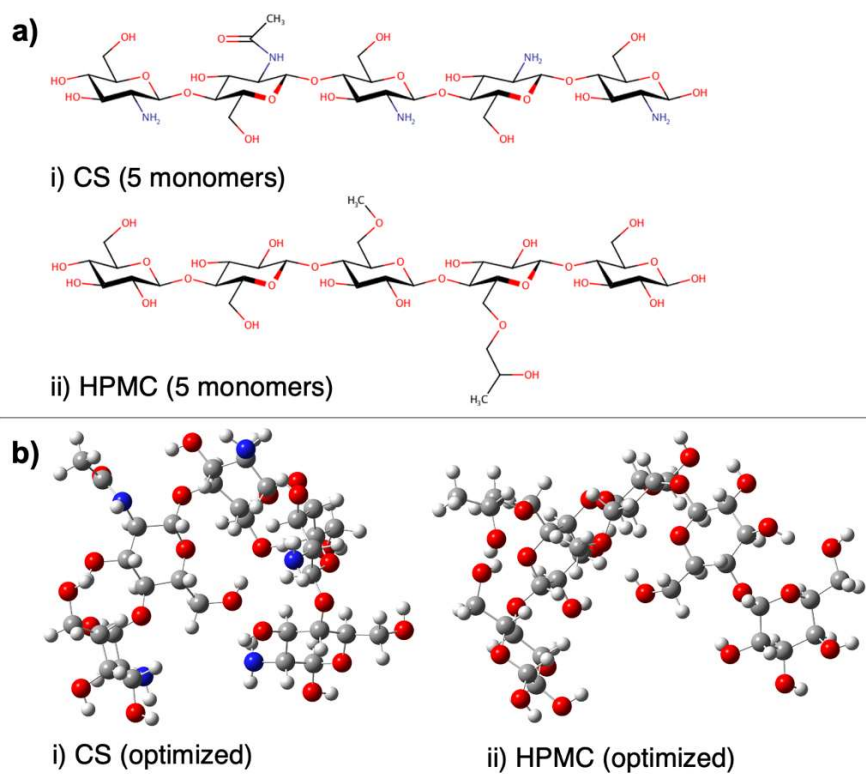


Figure S3. Schematic representation of **a)** initial and **b)** optimized molecular models of chitosan (CS) and hydroxypropyl methylcellulose (HPMC), consisting of 5 monomeric units in each case. Notice how both polymeric chains contract after the optimization of their geometries (B3LYP/6-311G(d,p)). (Color legend: Carbon = gray; Hydrogen = white; Oxygen = red; and Nitrogen = blue).

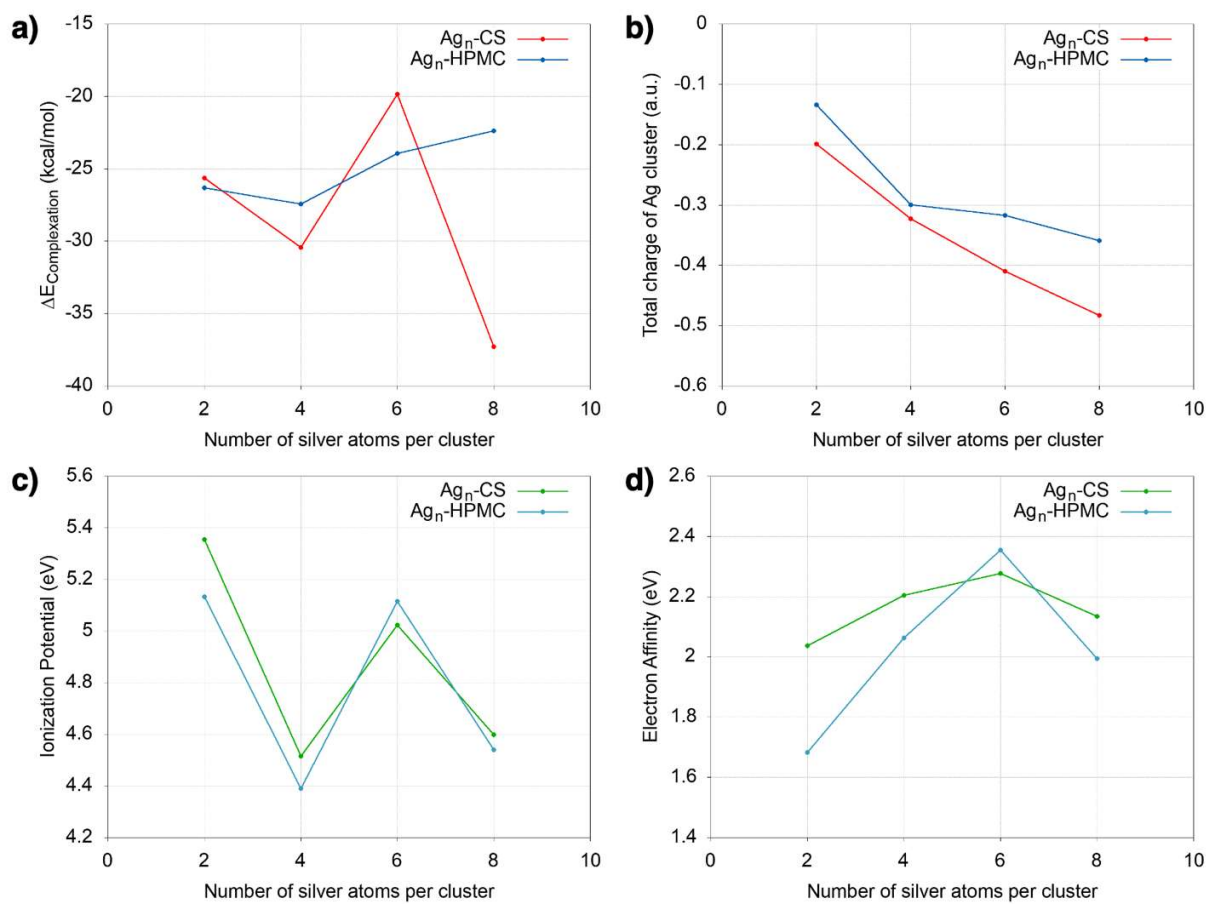


Figure S4. Plots of **a)** $\Delta E_{\text{complexation}}$, **b)** total charge of silver clusters, **c)** ionization potential (IP), and **d)** electron affinity (EA) of the $\text{Ag}_n\text{-CS/HPMC}$ complexes in the function of silver atoms per cluster.