Supplementary Information

Interfacial synergy between biogenic silica and reduced graphene oxide: Experimental and theoretical insights into cationic pollutants adsorption

Mayara Bitencourt Leão[a], Mônica Carla Lopes[b], Laura F. O. Vendrame[c] , Leonardo Costa Dias[a], Ivana Zanella[c], Solange B. Fagan,[c] Robert Burrow[b], Iuri Medeiros Jauris[d], Carolina Ferreira de Matos Jauris[b*]

[a]Environmental Science and Technology Center, Campus Caçapava do Sul, Federal University of Pampa, Caçapava do Sul, Brazil,
[b]Chemistry Department, Federal University of Santa Maria, Santa Maria, Brazil,
[c]Physics Department, Franciscan University, Santa Maria, Brazil,
[d]School of Sciences, Pontifical Catholic University of Rio Grande do Sul, Porto Alegre, Brazil

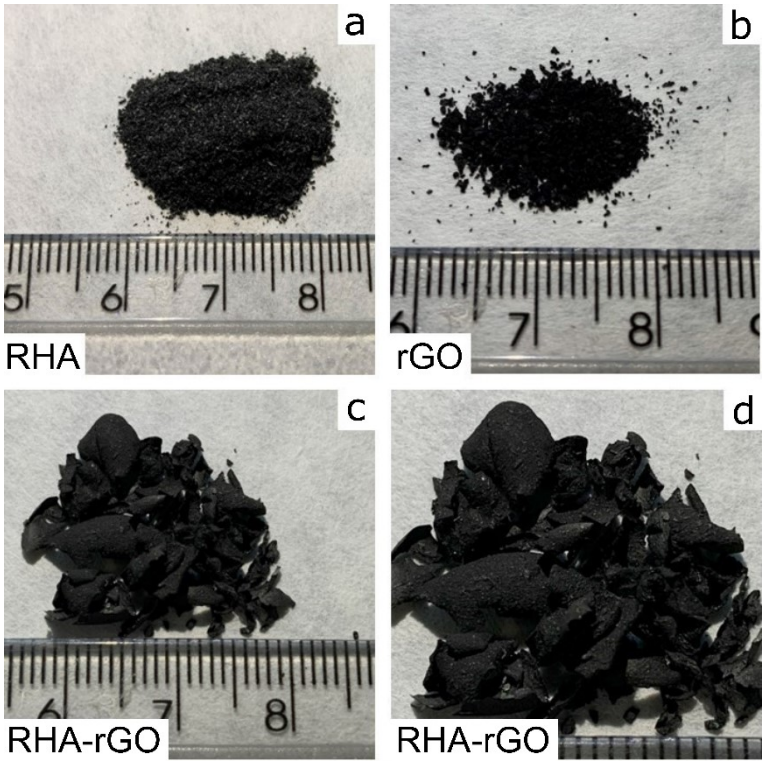

Figure S1. Digital photographs of the materials after drying: (a) rice husk ash (RHA), (b) reduced graphene oxide (rGO), and (c,d) RHA–rGO nanocomposite. The images illustrate the macroscopic appearance of the samples, highlighting the fine, powder-like morphologies of RHA and rGO, and the formation of larger, compact agglomerates in the hybrid material.

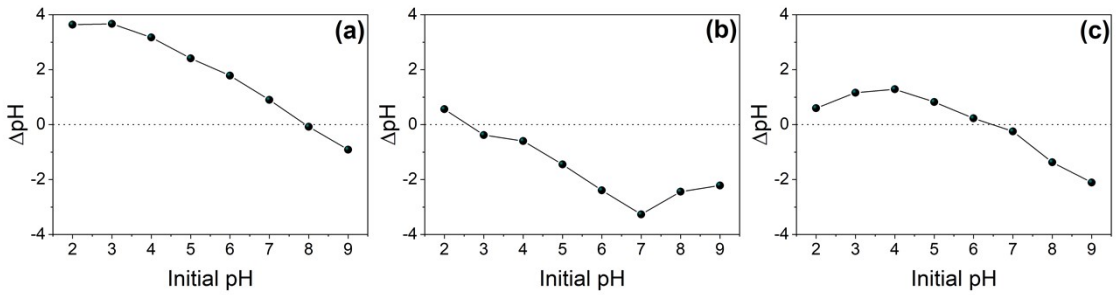

Figure S2. Point of zero charge for (a) rice husk ash, (b) reduced graphene oxide, and (c) nanocomposite of rice husk ash and reduced graphene oxide.

Table S1. FTIR band assignments and mechanistic relevance for GO, rGO, RHA, and RHA–rGO before and after Safranin O adsorption. The table lists key wavenumber ranges (cm^{-1}), band assignments, the main samples where they are observed, and the spectral changes upon dye uptake, highlighting Si–O–C interfacial coupling, π–active domains, and hydrogen-bond/electrostatic contributions to the proposed mechanism.

Band (cm^{-1})	**Assignment**
~3400	O-H ν_s (of surface -OH / physisorbed H_2O)
~1720	C=O ν_s (carboxyl/ketone from oxidation)
~1630	H-O-H bending (adsorbed water) aromatic C=C contribution
1610 to 1500	Aromatic C=C / C=N (Safranin O phenazinium ring)
1250 to 1050	C-O-C / C–O stretching (epoxide/hydroxyl)
1080 to 1030	Si-O-Si ν_{as}(silica network)
~ 800	Si-O-Si ν_s
~ 470	Si–O $_{bending}$
1100–1000	Si–O–C interfacial linkage (silica–carbon coupling)

Table S2. Raman parameters for GO, rGO, RHA, and RHA-rGO samples, including D and G band positions, I_D/I_G ratios, and the calculated in-plane crystallite (L_a) and defect (L_D) domain sizes, used to assess structural order and defect density after reduction and hybridization.

Amostra	**D band (cm^{-1})**	**G band (cm^{-1})**	**I_D/I_G**	**L_a (nm)**	**L_D (nm)**
RHA	1336	1599	1.263	15.2	179.5
RHA-rGO	1332	1569	1.550	12.4	163.4
rGO	1339	1567	1.403	13.7	170.4
GO	1341	1580	0.995	19.3	203.8

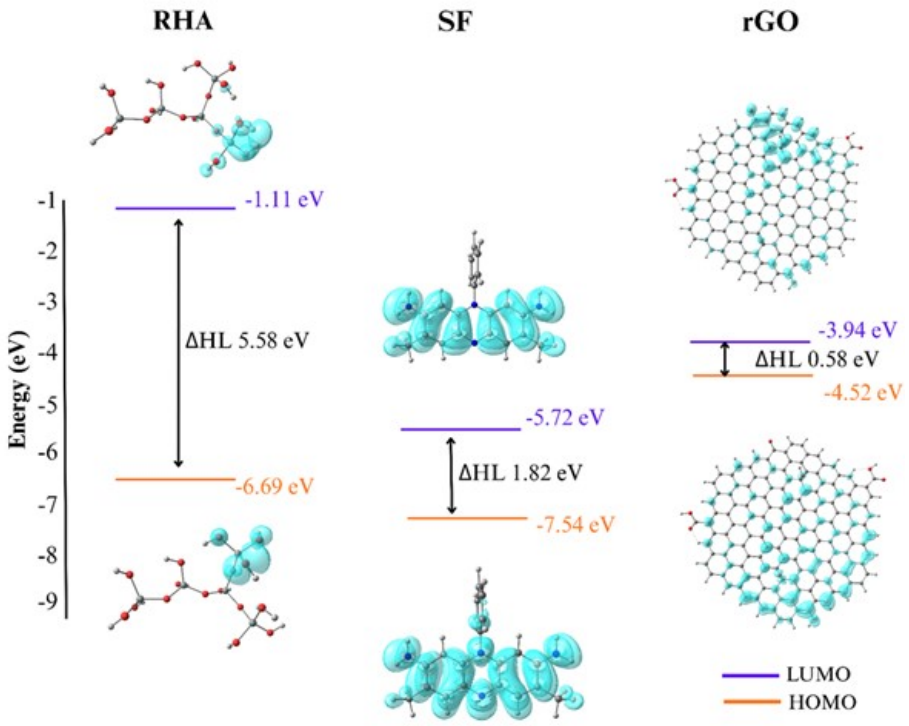

Figure S3: Schematic representation of Frontier Molecular Orbital energy diagram of RHA, SF and rGO. Orbital charge density isosurface value of 0.0006 e^{-} $Å^{-3}$.

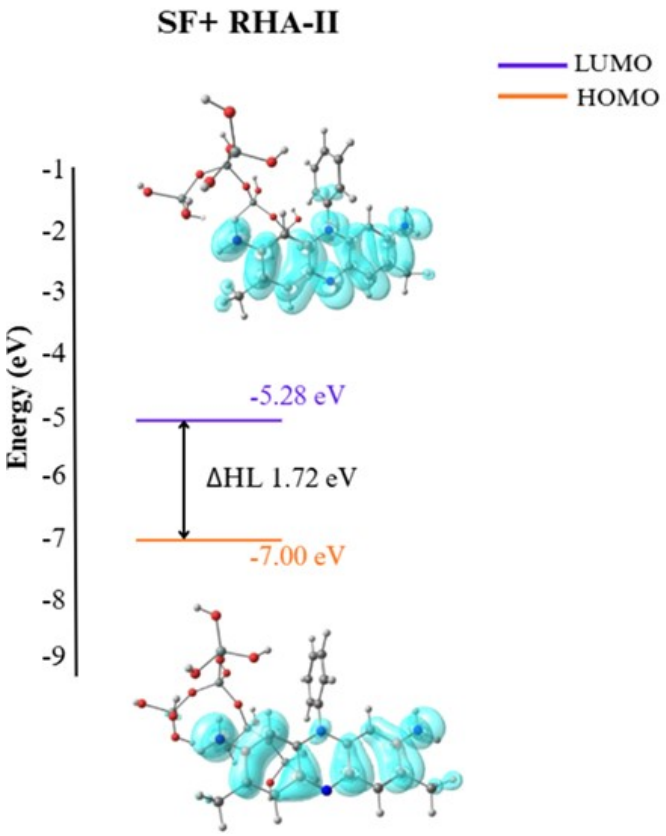

Figure S4. Energy diagram of SF+RHA-II, the most stable configuration among all those studied for SF+RHA. Orbital charge density isosurface value of 0.0006 e^{-} $Å^{-3}$.

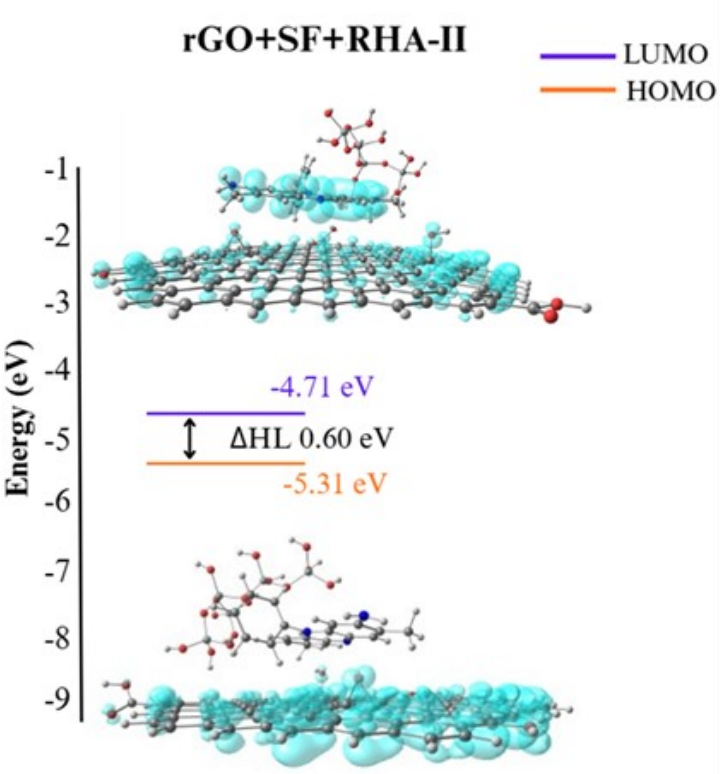

Figure S5 - Energy diagram of rGO+SF+RHA-II, the most stable configuration among all those studied for of rGO+SF+RHA. Orbital charge density isosurface value of 0.0006 e^{-} $Å^{-3}$.