Supporting information

For

Adsorption and coadsorption of single and multiple natural organic matter on Ag (111) surface: A DFT-D study

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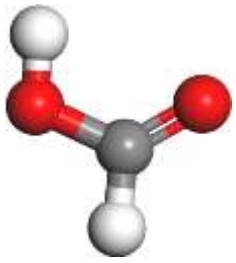
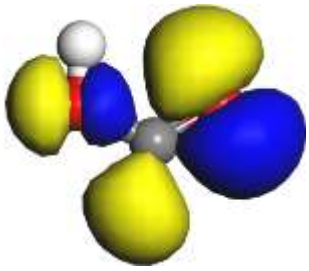
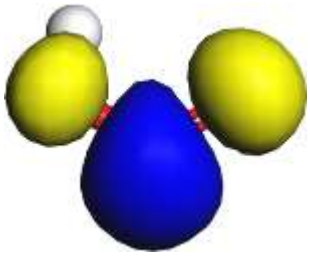
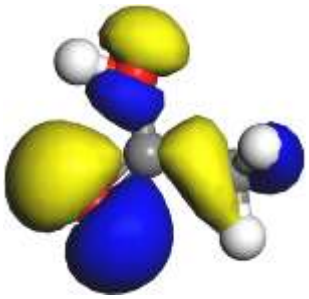
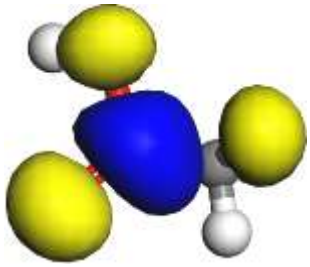
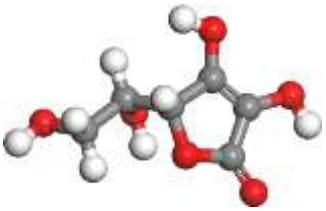
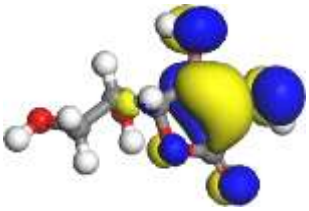
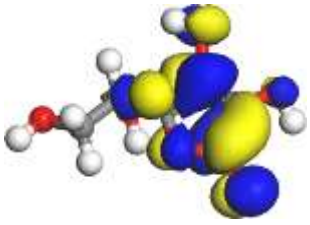
DFT-D Gas phase		
Adsorbate	**HOMO**	**LUMO**
Formic acid 		
Acetic acid 		
Ascorbic acid 		

Figure S1: Optimized structures and the frontier molecular orbital density distributions (HOMO and LUMO in gas phase.

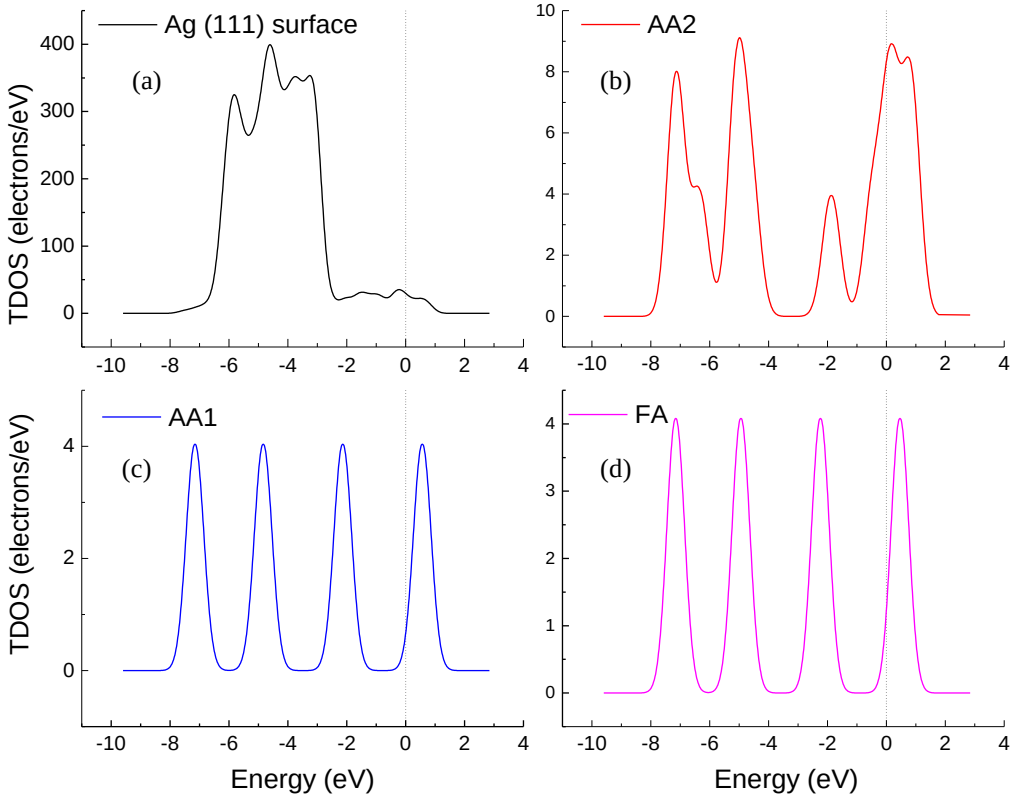


Figure S2: Total density of states in the gas phase for (a) Ag (111) surface (b) AA2, (c) AA1 and (d) FA.

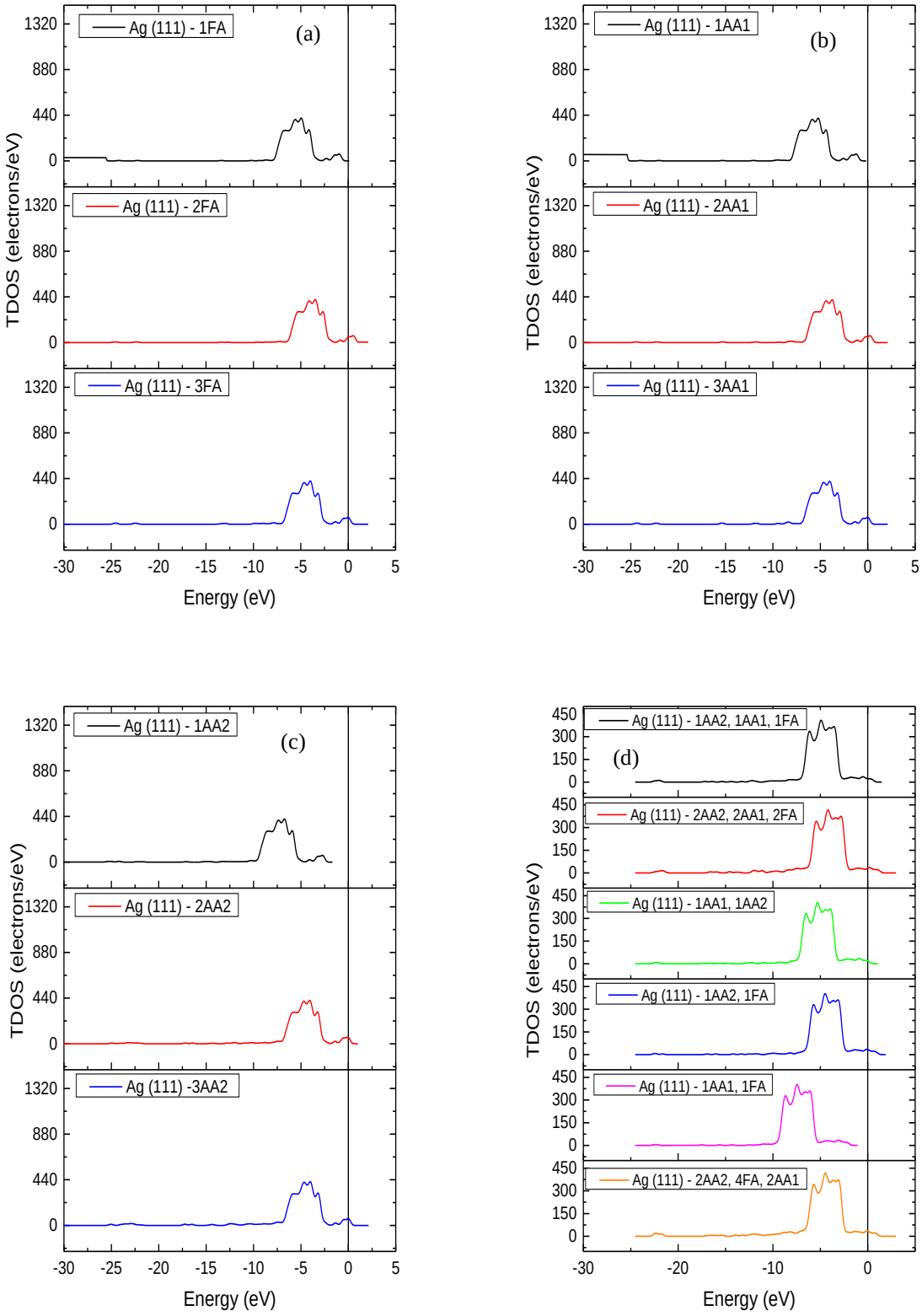


Figure S3: The total density of states (TDOS) in the gas phase for (a) Ag (111) - 1FA, Ag (111) – 2FA and Ag (111) – 3FA (b) Ag (111) – 1AA1, Ag (111) – 2AA1 and Ag (111) – 3AA1 (c) Ag (111) – 1AA2, Ag (111) – 2AA2 and Ag (111) – 3AA2 and (d) Ag (111) surface with a mixture of NOM's. The Fermi level is indicated with a black vertical line.

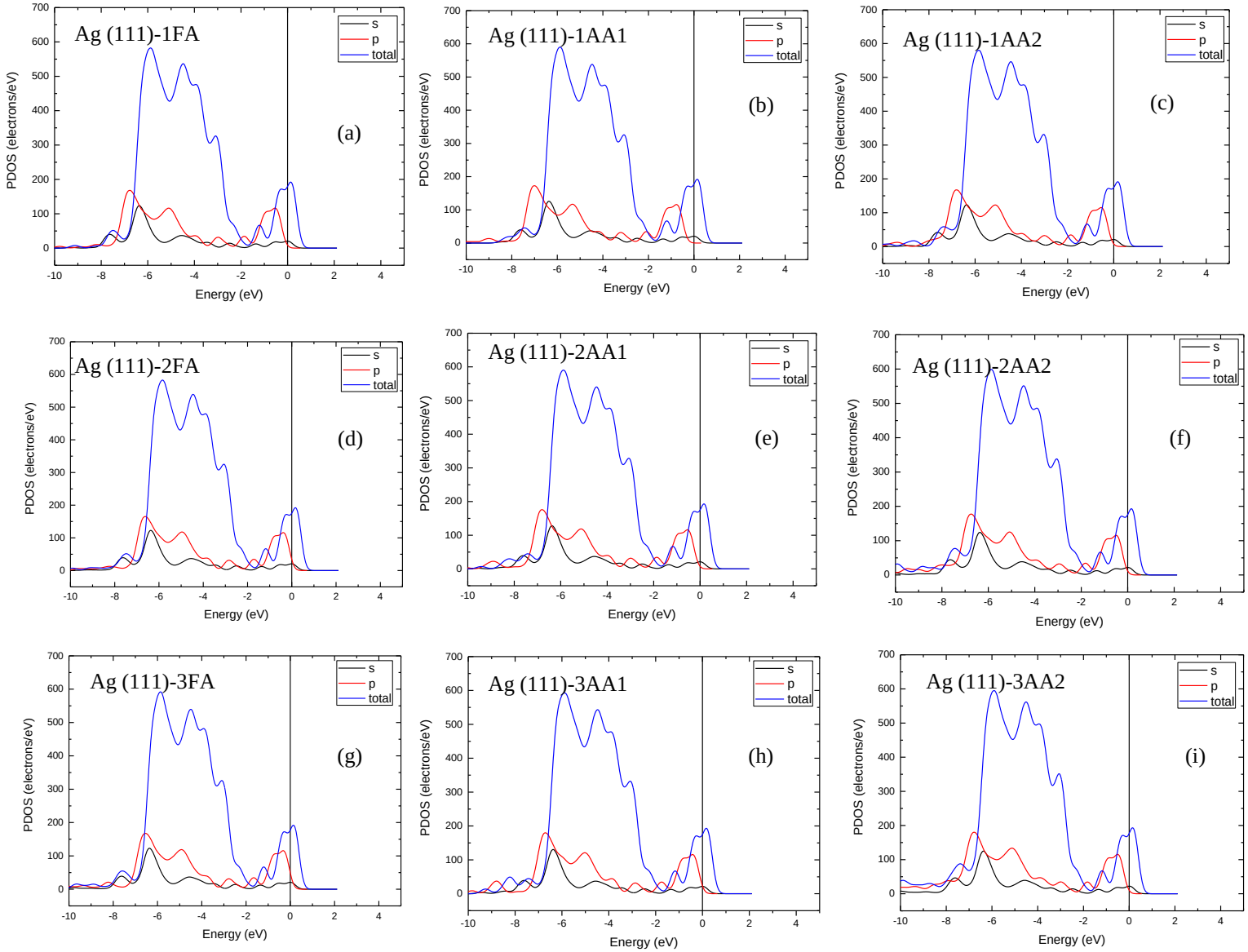


Figure S4: Projected density of states of NOM's on Ag (111) surface (a-i) in gas phase using DFT-D/GGA level of theory.

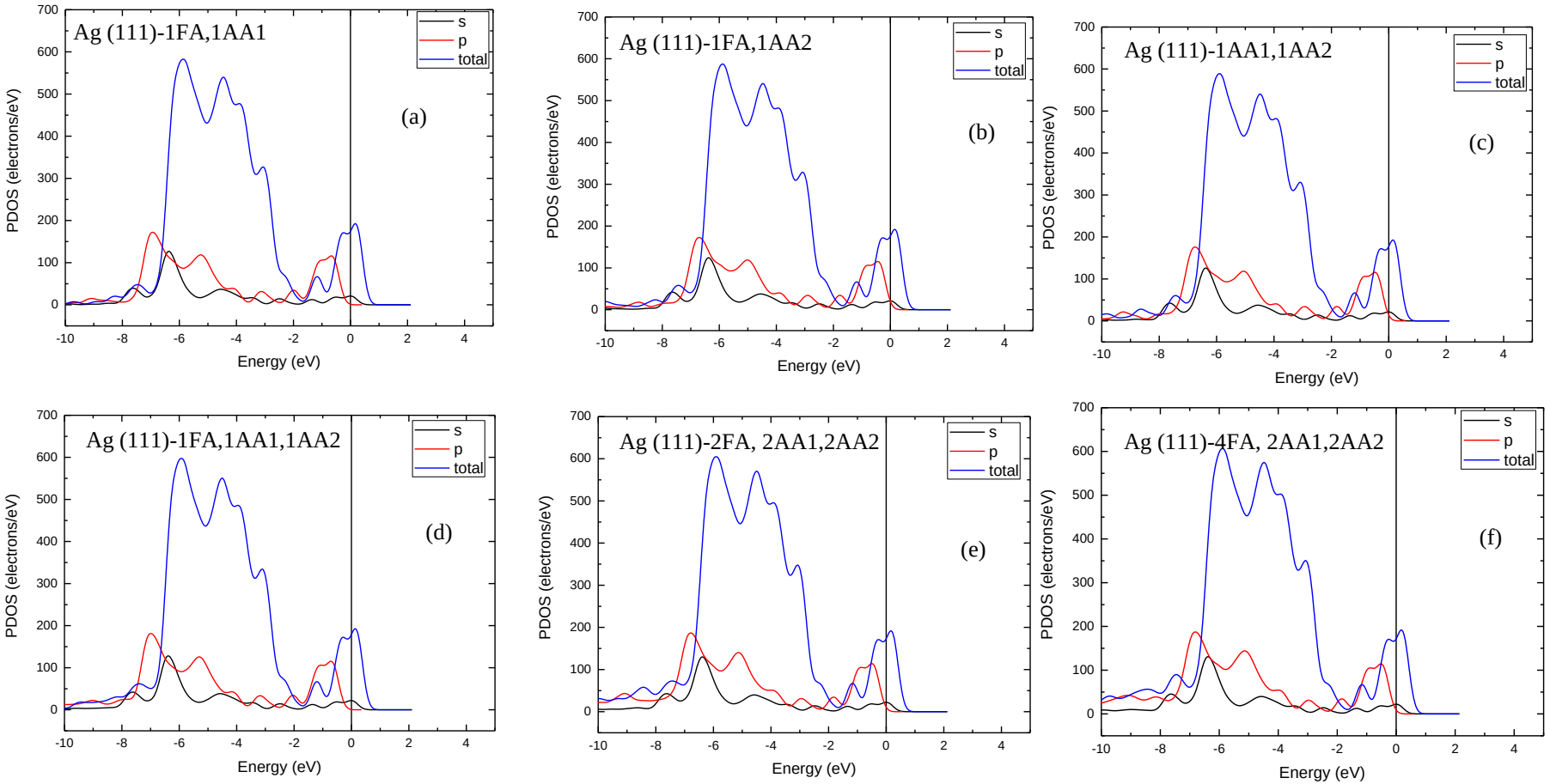


Figure S5: Projected density of states of NOM's on Ag (111) surface (a-f) in gas phase using DFT-D/GGA level of theory.