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Remarkable hole transport properties of Spiro[fluorene-9,9'-xanthene] derivatives containing natural aminoacid substituents for perovskite photovoltaics

Hosein Askari,[a] Zahra Shariatinia,*[,a] Saeedeh Sarabadani-Tafreshi,[a] Nora H. de Leeuw[b]

[a]Department of Chemistry, Amirkabir University of Technology (Tehran Polytechnic),

P.O.Box:15875-4413, Tehran, Iran.

[b]School of Chemistry, University of Leeds, LS2 9JT Leeds, UK

[c]Department of Earth Sciences, Utrecht University, 3584 CB Utrecht, The Netherlands

*Corresponding author.
E-mail: shariati@aut.ac.ir

Table S1. HOMO, LUMO, and E_g values of HTMs containing natural amino acid substituents attached to ortho positions of aromatic rings of SFX core via oxygen atom of COOH group in dichloromethane solvent.

HTM	E(HOMO) (eV)	E(LUMO) (eV)	E_g (eV)
SFX-Alanine	-5.881	-1.274	4.607
SFX-Arginine	-5.921	-1.253	4.668
SFX-Asparagine	-5.936	-1.266	4.670
SFX-Aspartic acid	-5.853	-1.245	4.608
SFX-Cysteine	-5.952	-1.325	4.627
SFX-Glutamic acid	-5.864	-1.232	4.632
SFX-Glutamine	-5.792	-1.238	4.554
SFX-Glycine	-5.853	-1.245	4.608
SFX-Histidine	-5.972	-1.296	4.676
SFX-Isoleucine	-5.980	-1.270	4.710
SFX-Leucine	-5.898	-1.269	4.629
SFX-Lysine	-5.874	-1.271	4.603
SFX-Methionine	-5.861	-1.300	4.561
SFX-Phenylalanine	-5.967	-1.284	4.683
SFX-Proline	-5.868	-1.241	4.627
SFX-Selenocysteine	-5.794	-5.409	0.385
SFX-Serine	-5.930	-1.285	4.645
SFX-Threonine	-5.941	-1.281	4.660
SFX-Tryptophan	-5.317	-1.267	4.050
SFX-Tyrosine	-5.729	-1.088	4.641
SFX-Valine	-5.893	-1.265	4.628

Table S2. HOMO, LUMO, and E_g values of HTMs containing natural amino acid substituents attached to meta positions of aromatic rings of SFX core via oxygen atom of COOH group in dichloromethane solvent.

HTM	E(HOMO) (eV)	E(LUMO) (eV)	E_g (eV)
SFX-Alanine	-5.849	-1.296	4.553
SFX-Arginine	-5.844	-1.226	4.618
SFX-Asparagine	-5.863	-1.015	4.848
SFX-Aspartic acid	-5.852	-1.349	4.503
SFX-Cysteine	-5.879	-1.359	4.520
SFX-Glutamic acid	-5.854	-1.312	4.542
SFX-Glutamine	-5.871	-1.286	4.585
SFX-Glycine	-5.819	-1.260	4.559
SFX-Histidine	-5.910	-1.280	4.630
SFX-Isoleucine	-5.901	-1.212	4.689
SFX-Leucine	-5.837	-1.277	4.560
SFX-Lysine	-5.781	-1.268	4.513
SFX-Methionine	-3.996	-2.822	1.174
SFX-Phenylalanine	-5.887	-1.262	4.625
SFX-Proline	-5.805	-1.240	4.565
SFX-Selenocysteine	-5.589	-5.424	0.165
SFX-Serine	-5.858	-1.308	4.550
SFX-Threonine	-5.882	-1.302	4.580
SFX-Tryptophan	-5.386	-1.204	4.182
SFX-Tyrosine	-5.861	-1.228	4.633
SFX-Valine	-5.897	-1.240	4.657

Table S3. HOMO, LUMO, and E_g values of HTMs containing natural amino acid substituents attached to para positions of aromatic rings of SFX core via oxygen atom of COOH group in dichloromethane solvent.

HTM	E(HOMO) (eV)	E(LUMO) (eV)	E_g (eV)
SFX-Alanine	-4.028	-2.894	1.134
SFX-Arginine	-5.805	-1.439	4.366
SFX-Asparagine	-5.827	-1.166	4.661
SFX-Aspartic acid	-1.945	-1.080	0.865
SFX-Cysteine	-4.892	-2.504	2.388
SFX-Glutamic acid	-5.913	-1.288	4.625
SFX-Glutamine	-3.741	-2.167	1.574
SFX-Glycine	-4.992	-2.158	2.834
SFX-Histidine	-5.768	-1.182	4.586
SFX-Isoleucine	-3.826	-2.804	1.022
SFX-Leucine	-5.924	-1.312	4.612
SFX-Lysine	-5.811	-1.147	4.664
SFX-Methionine	-5.815	-1.183	4.633
SFX-Phenylalanine	-4.315	-2.818	1.497
SFX-Proline	-5.889	-1.255	4.634
SFX-Selenocysteine	-4.349	-3.332	1.018
SFX-Serine	-3.479	-2.800	0.679
SFX-Threonine	-3.896	-2.421	1.476
SFX-Tryptophan	-3.100	-2.030	1.071
SFX-Tyrosine	-4.188	-2.345	1.844
SFX-Valine	-3.568	-2.094	1.474

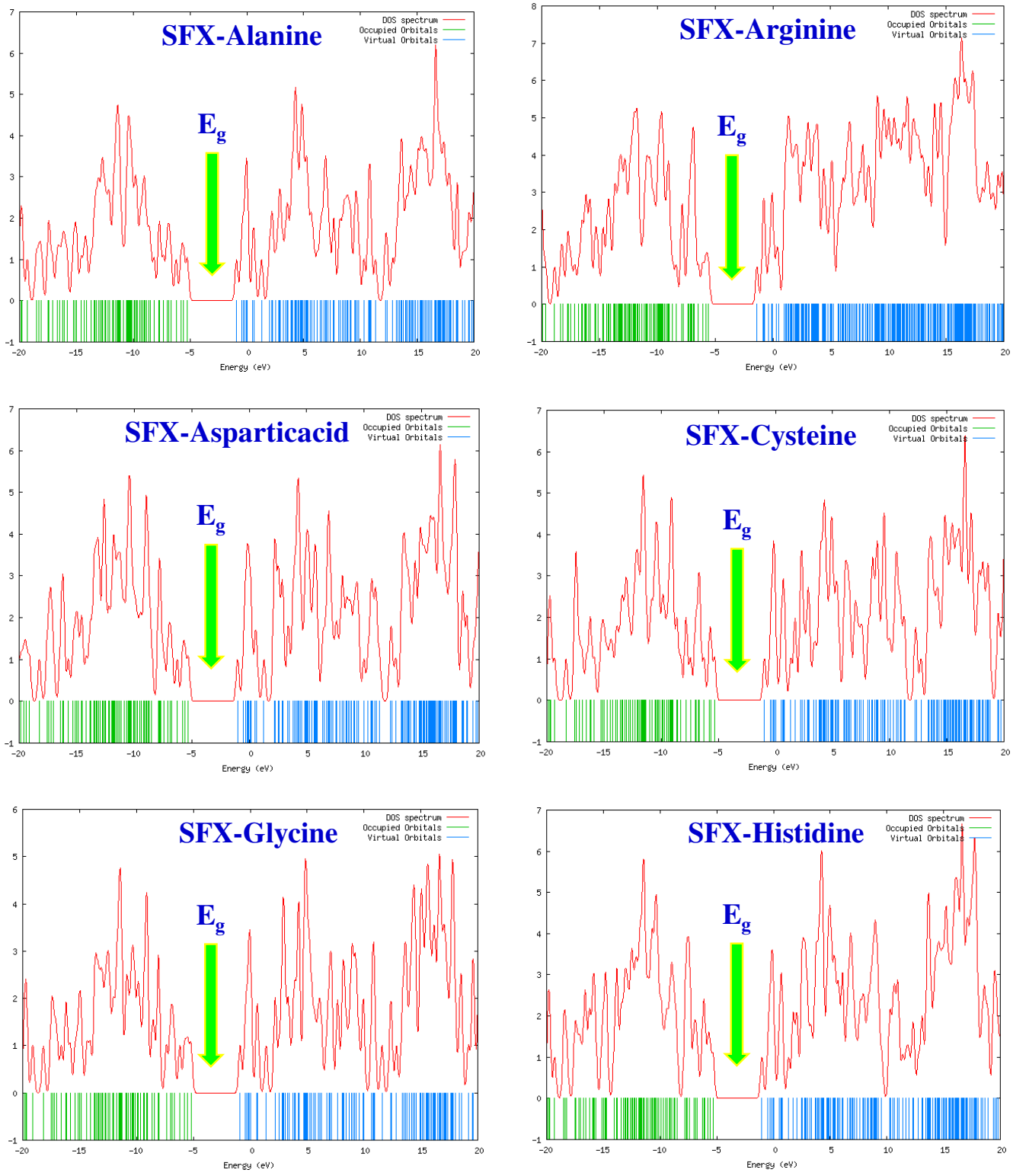
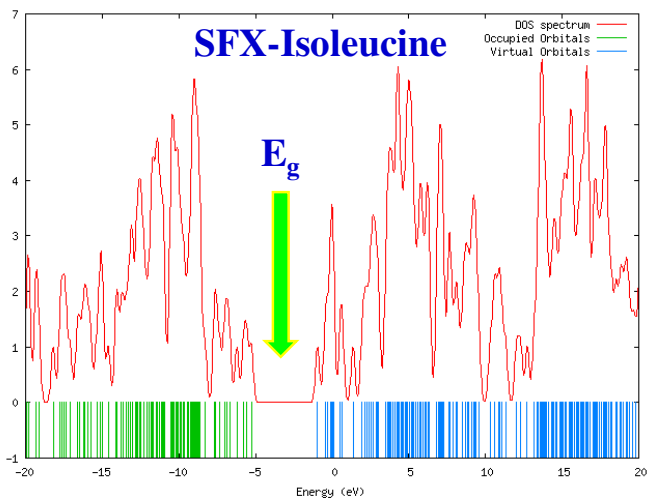
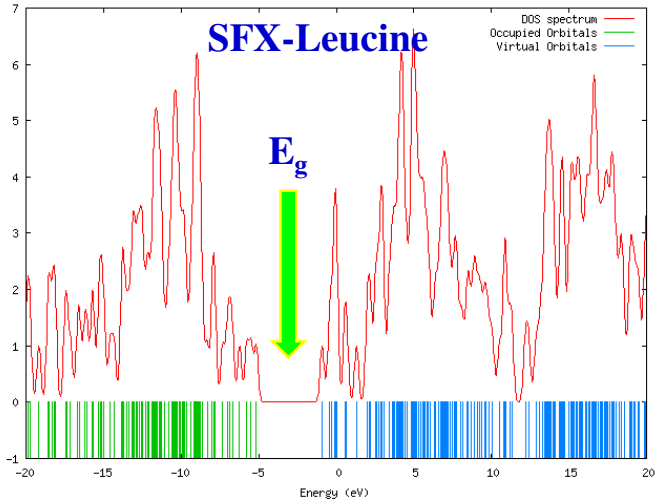
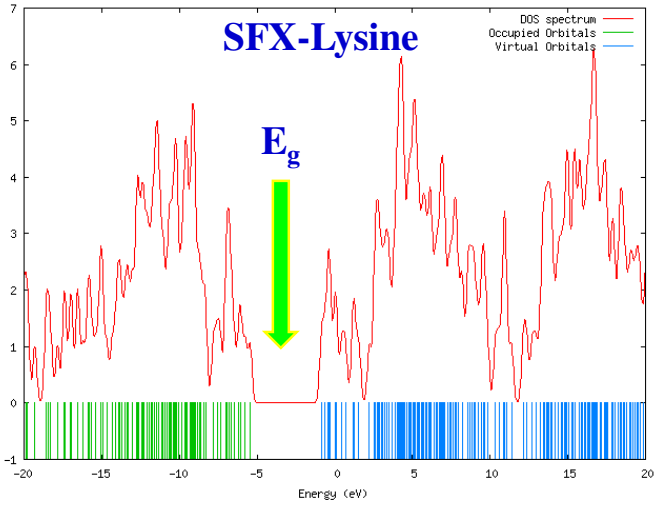
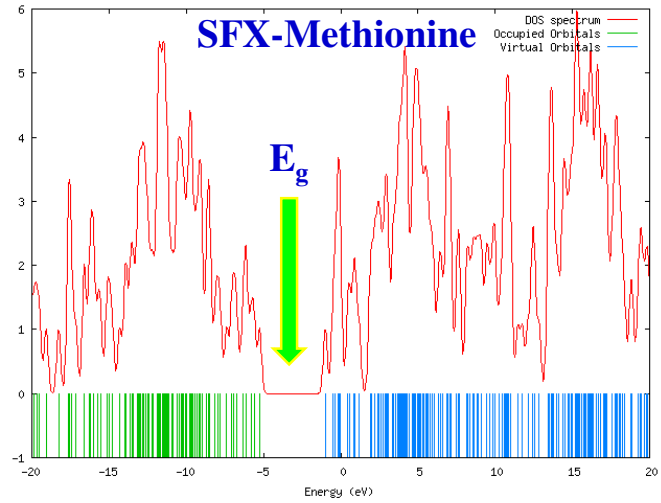


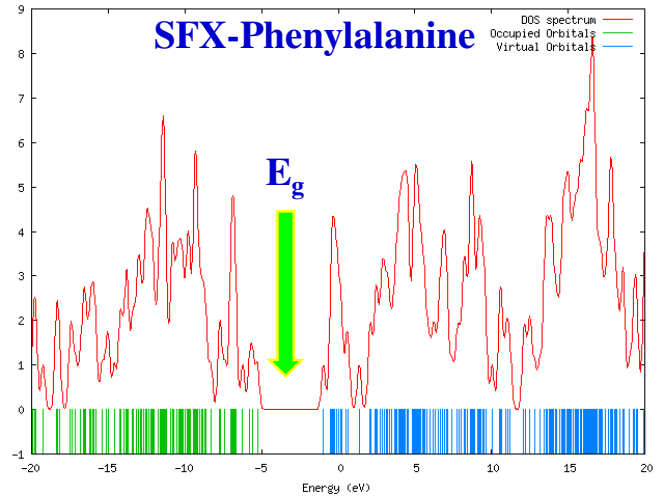
Fig. S1. The DOS spectra of SFX-based HTMs.











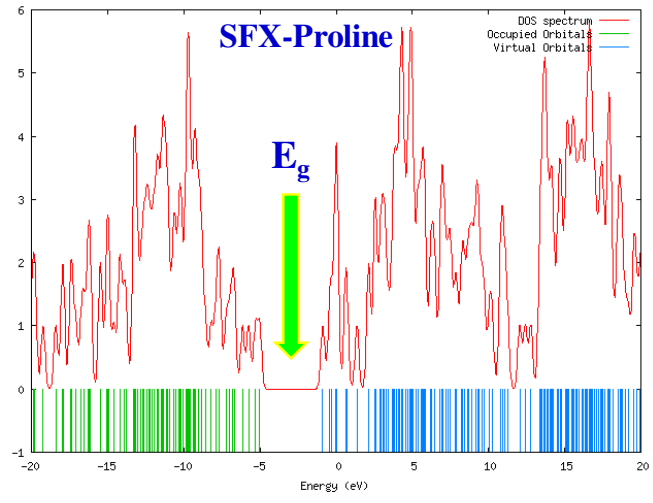
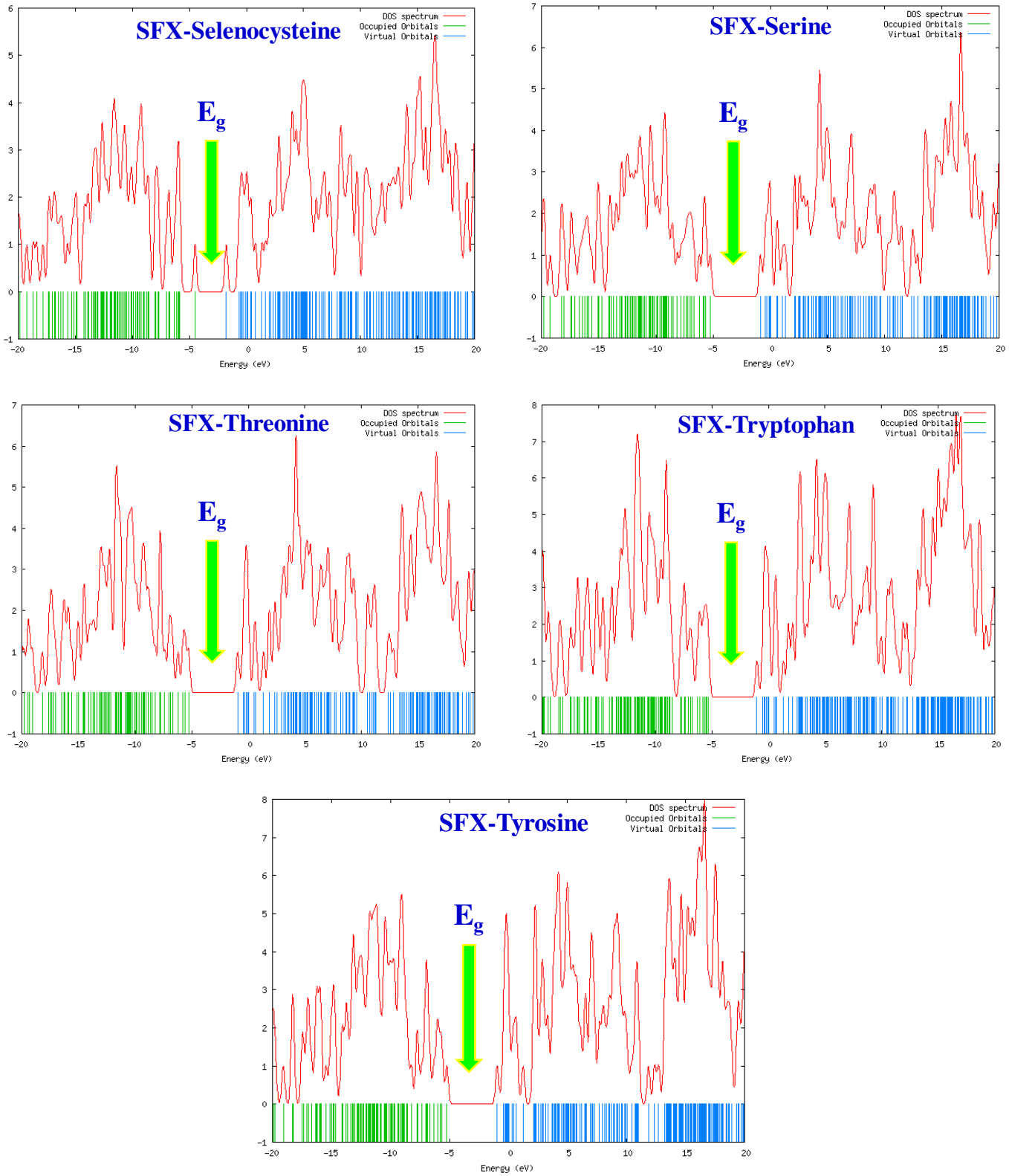


Fig. S1. Continued.



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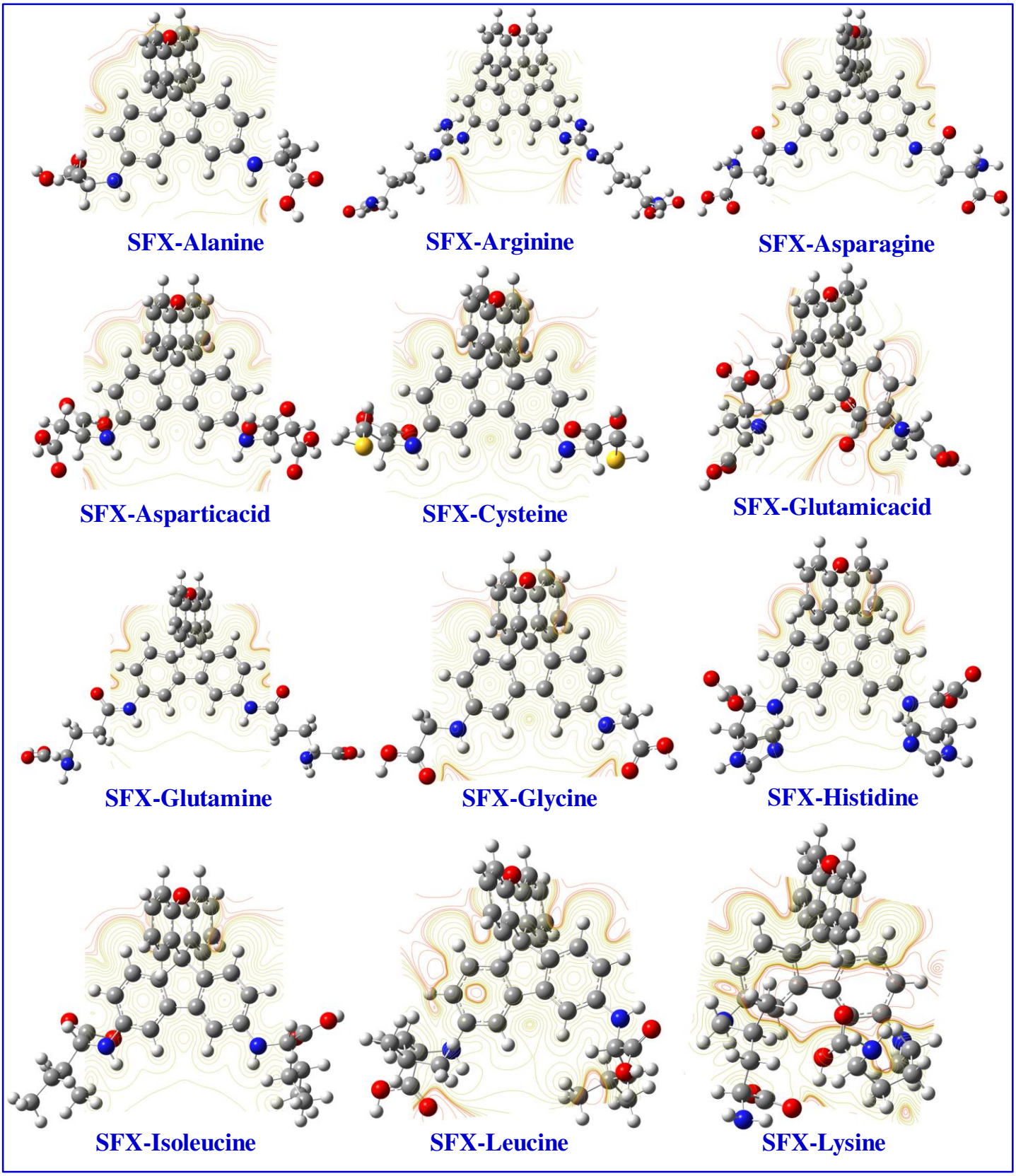
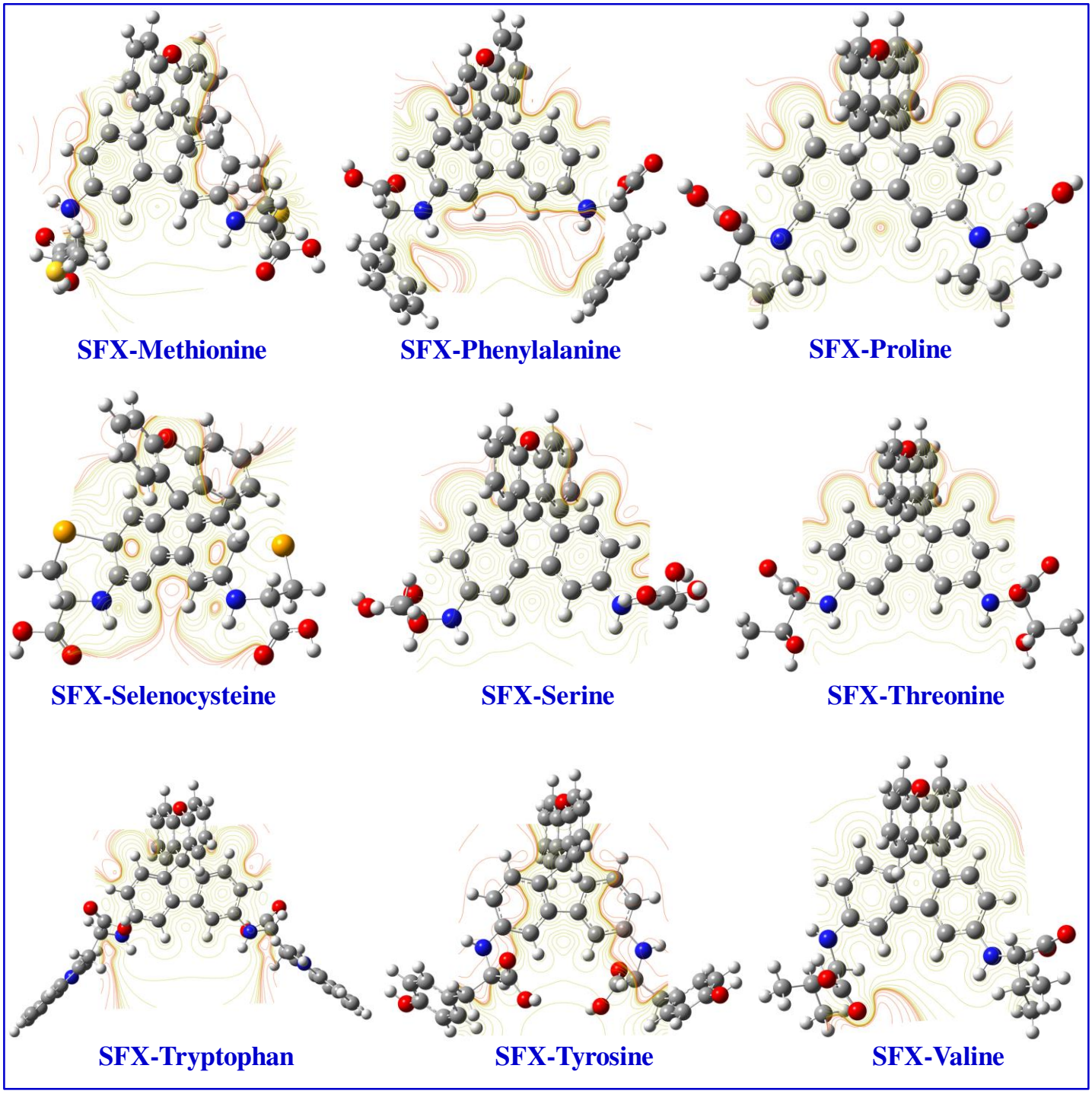


Fig. S2. The contour maps of SFX-based HTMs.



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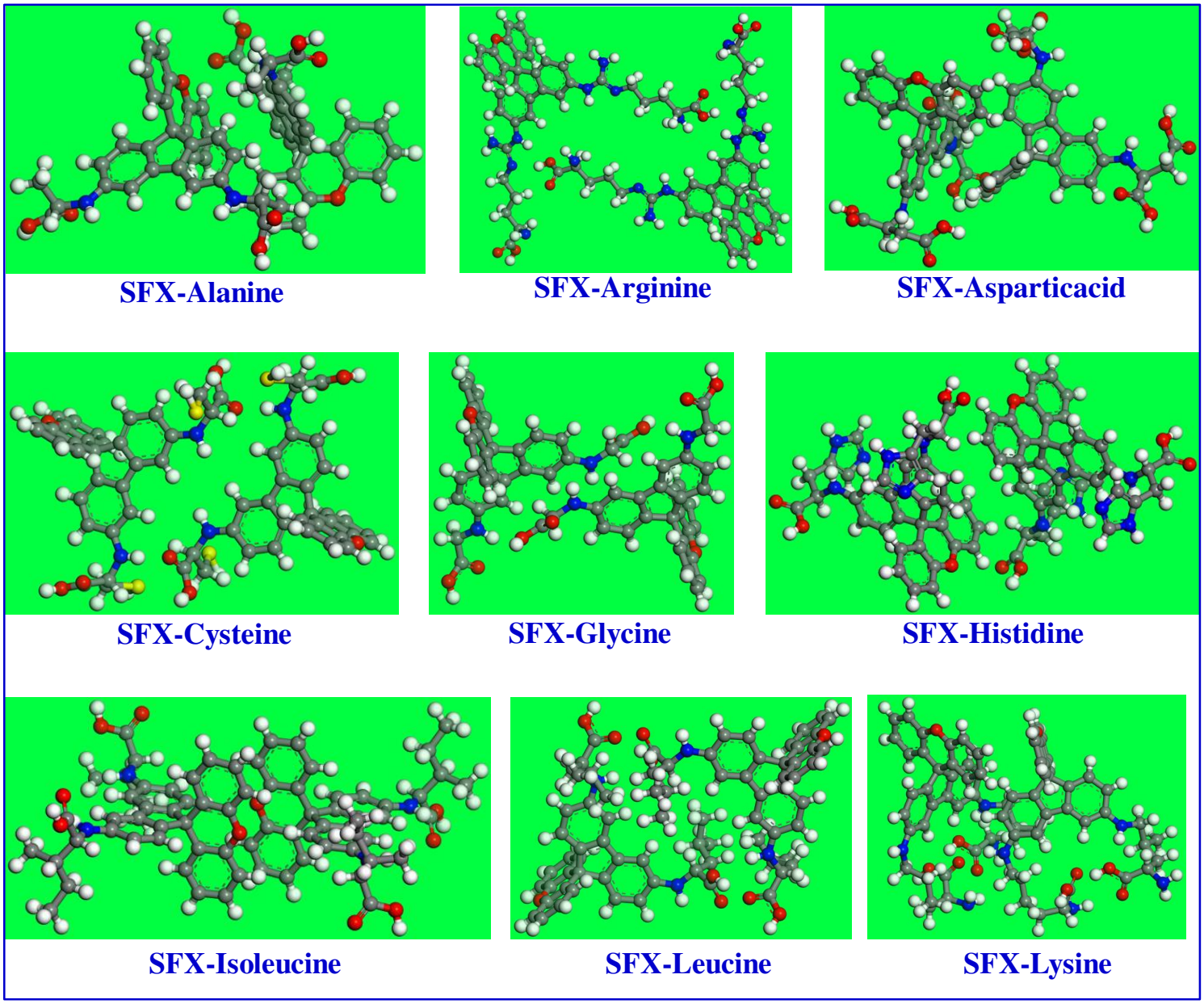

Fig. S3. Dimer structures of SFX-based HTMs used for hole mobility calculations.

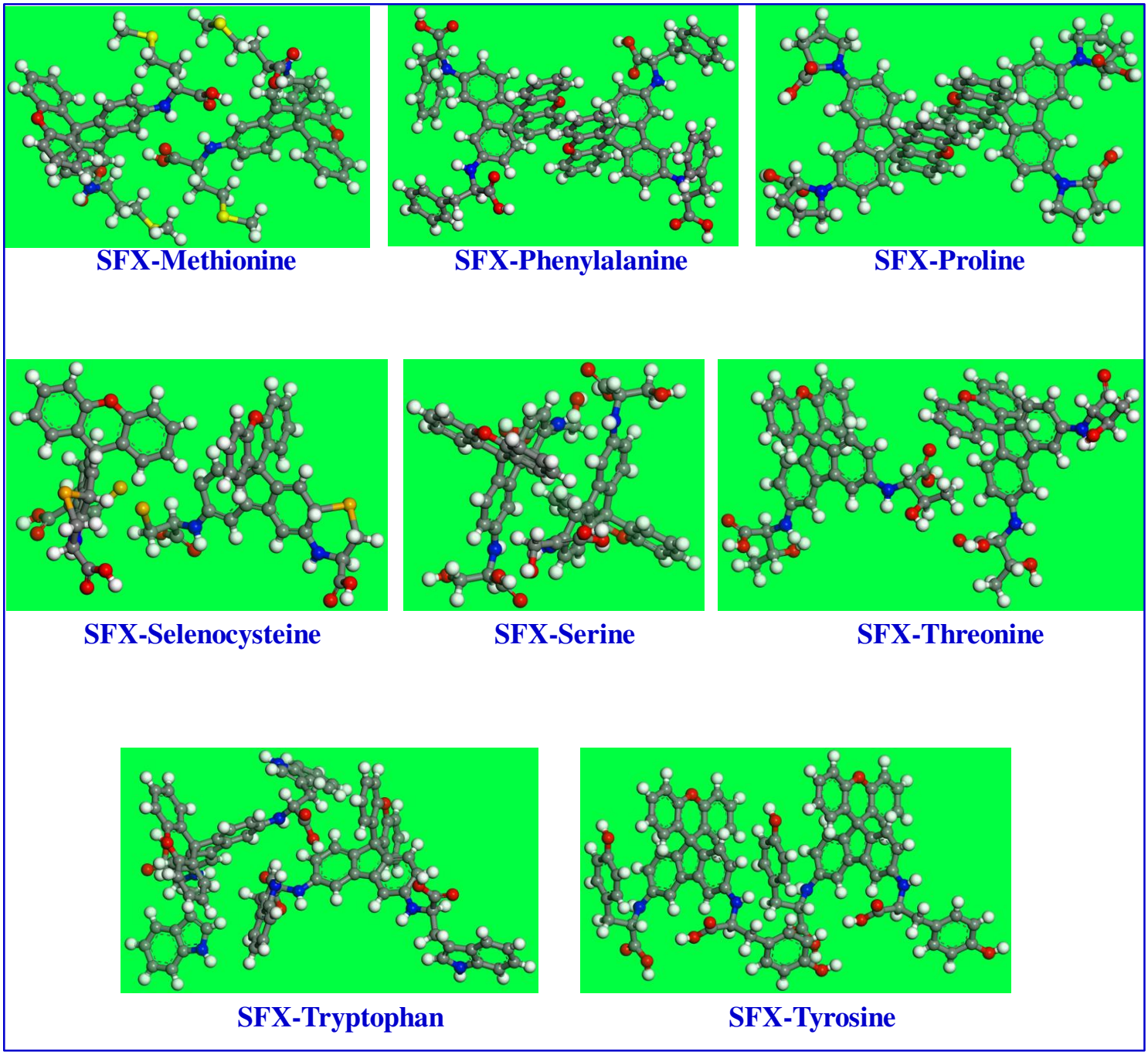

Fig. S3. Continued.