Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Lebedev et al. "Effect of Iron Doping…". Supporting Information

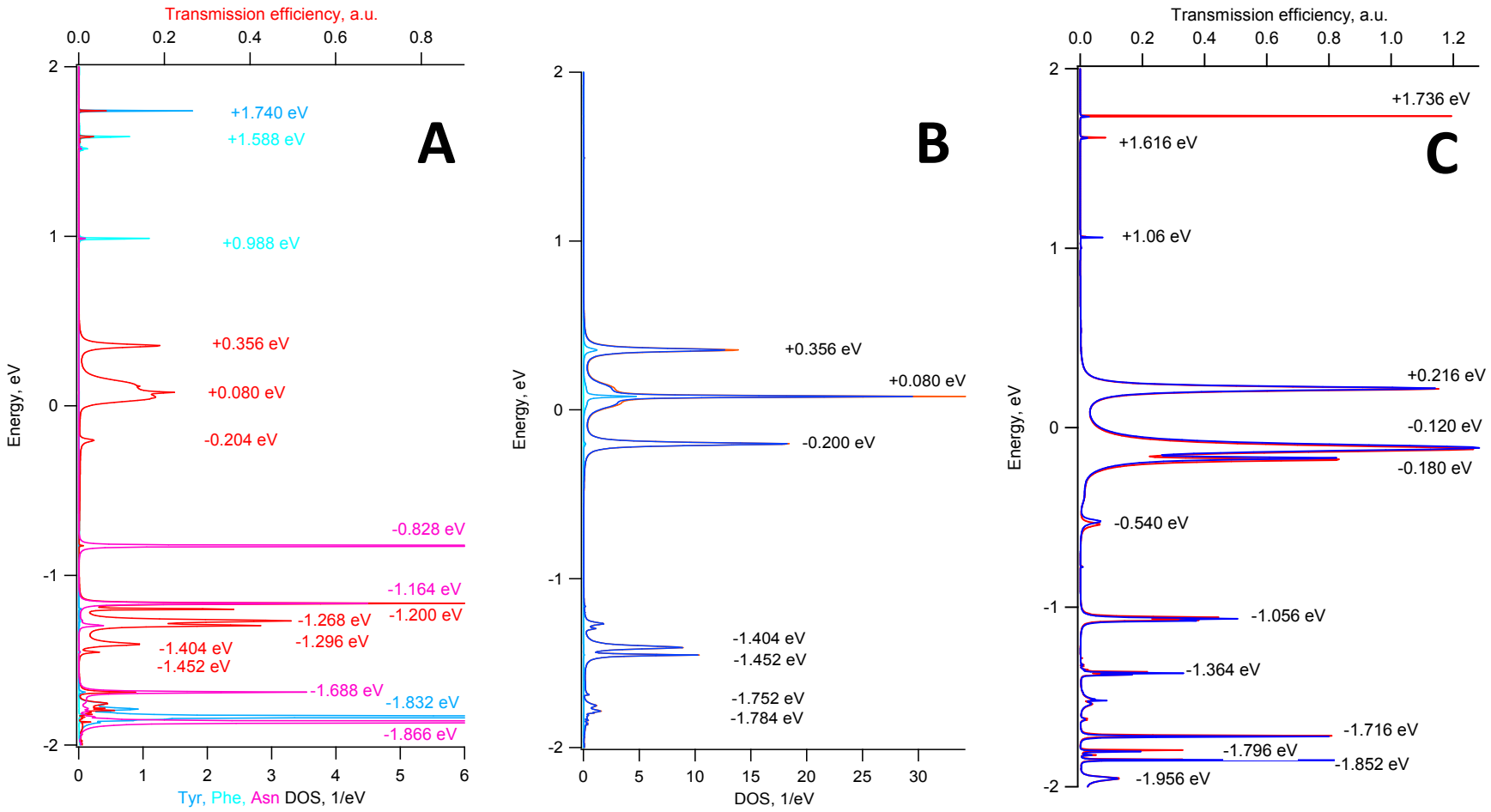

Figure S1. (A) Projected DOS (bottom scale) of charged Asn (-) and aromatic amino acids Phe (-) and Tyt (-), along with device ETS (top scale). Note the difference in DOS scales in all three graphs. (B) Projected DOS of s (-), p (-) and d (-) orbitals of FeS cluster along with its total FeS DOS (-). (D) The effect of temperature (300K vs 100K) on Rd ETS at bias = +/-0.5V.

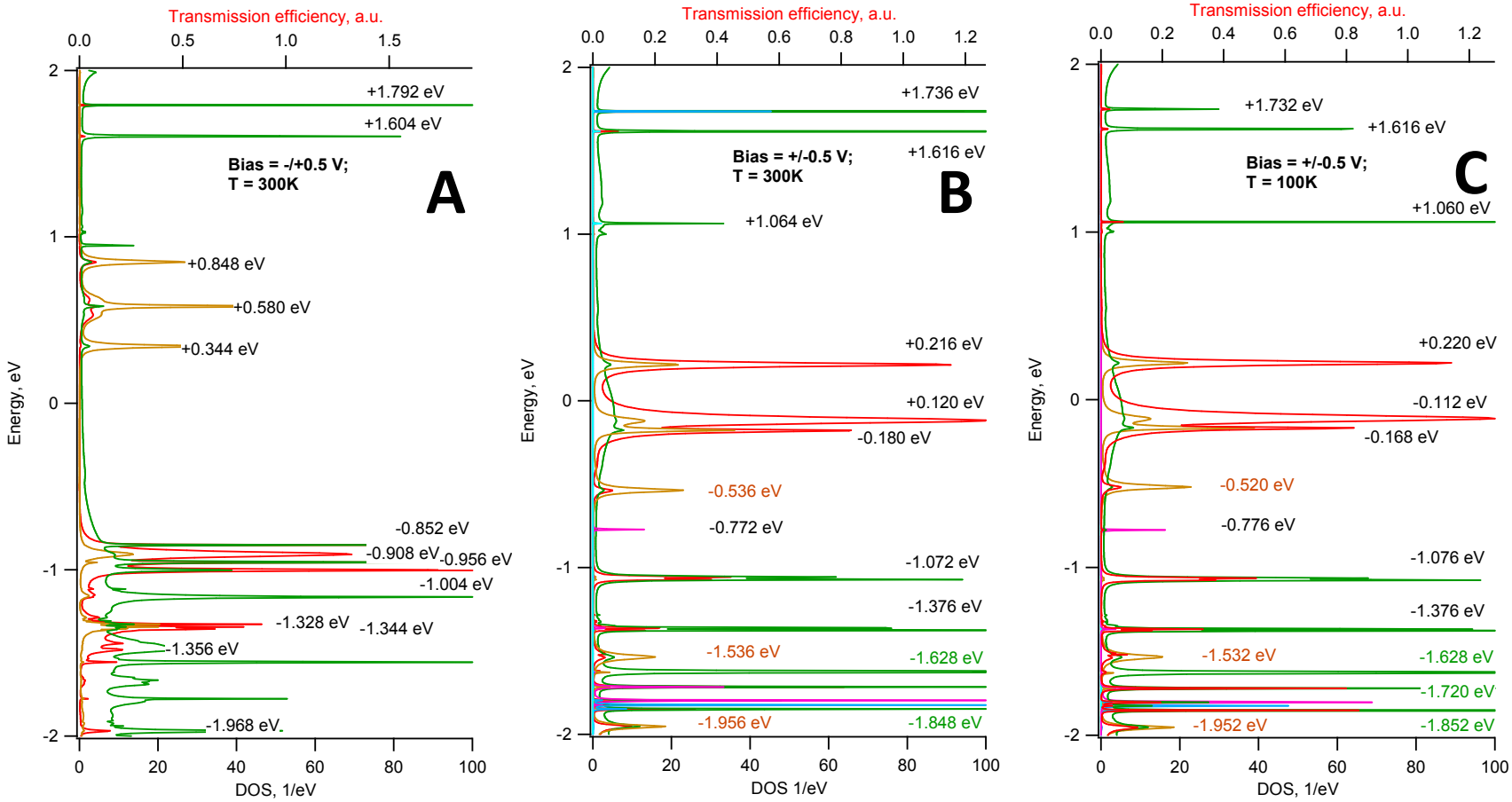

Figure S2. Projected DOS (bottom scale) of FeS cluster, Rd backbone, charged Asn (-) and aromatic amino acids Phe (-) and Tyt (-), along with device ETS (top scale) at bias voltage (A) -/+ 0.5V at 300K, (B) +/-0.5V at 300K and (C) +/-0.5V at 100K.

Table S1. Estimation of the number of channels contributing to the main transmission bands at B=0V; 300K. In **Bold** are transmission efficiencies with probability >0.1. [Conclusion: single path of ET in every main TRA band, including broad band around +0.080 eV.]

Energy (eV)	Transmission Efficiency, main Channel	Transmission Efficiency, secondary Channel
+1.740	0.06400441	0.0001603325
+1.588	0.03447419	0.00006422773
+0.356	**0.1882573**	**0.001165328**
+0.341	0.08004179	0.001370307
+0.132	**0.1246220**	**0.0005551498**
+0.0800	**0.2192663**	**0.004042517**
+0.073	**0.1748399**	**0.002022132**
+0.061	**0.1734434**	**0.0003919742**
+0.044	**0.1689674**	**0.0003059458**
-0.204	0.03520522	0.0005741136
-0.206	0.03370870	0.0005576384
-1.164	**0.8977457**	**0.003109691**
-1.200	**0.3482451**	**0.01344485**
-1.281	**0.1928708**	**0.02411418**
-1.404	**0.1416306**	**0.0001510471**
-1.688	**0.1327055**	**0.0003263575**

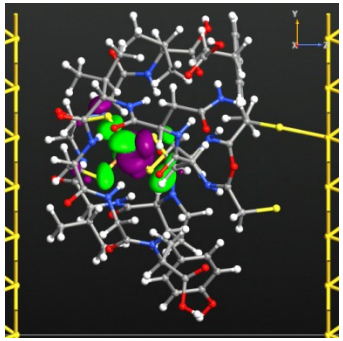

Figure S3. Spatial distribution of molecular transmission eigenstate at +0.032 eV (isovalue = 1.0; bias = 0; temperature 300K). Note: this eigenstate is similar to the eigenstate located in ETS at +0.136eV indicating that the broad band might be a single one, overlapping the narrow peak at 0.080 eV on both sides.