Supplementary Data

for

Ab-initio Investigation of Per- and Poly-fluoroalkyl substances (PFAS) Adsorption on Zerovalent Iron (Fe^0)

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The supplementary data provides 4 tables; the adsorption energies of PFBA and PFBS on Fe(111) and Fe(110), the adsorption energies of preadsorbed O on Fe(110), and the adsorption energies for preadsorbed Ni on Fe(110).

Tables

Table S1. Adsorption energies for PFBA and PFBS over different sites on Fe (111)

Molecule	Site	Adsorption Energy (Eads.) (eV)
PFBA	Fcc	-2.44
	Hcp	-0.77
	Hollow	**-2.50**
	Top	0.05
	Top-fcc	-1.17
	Top-hcp	-0.71
PFBS	Fcc	-2.92
	Hcp	**-3.51**
	Hollow	-3.04
	Top	-2.86
	Top-fcc	-3.39
	Top-hcp	-3.46

Table S2. Adsorption energies for PFBA and PFBS over different sites on Fe (110)

Molecule	Site	Adsorption Energy (Eads.) (eV)
PFBA	3-fold	-0.45
	Long Bridge	**-2.23**
	Short Bridge	-0.60
	Top	-0.43
PFBS	3-fold	**-3.56**
	Long Bridge	-2.21
	Short Bridge	-2.94

	Top	-3.39

Table S3. Adsorption energies for a pre-adsorbed oxygen monolayer for different adsorption sites over Fe (110).

Site	**Eads. (eV)**
3-fold	**-4.13**
Long Bridge	-2.85
Short Bridge	-2.79
Top	-1.63

Table S4. Adsorption energies for a pre-adsorbed Ni monolayer for different adsorption sites over Fe (110).

Site	**Eads. (eV)**
3-fold	0.30
Long Bridge	**-0.31**
Short Bridge	0.07
Top	0.75