

Supporting Information

		Hematite Face						
		(001)	(010)	(011)	(100)	(111)	(110)	(101)
AS Face	(001)	0.05	0.05	0.38	0.05	0.35	0.03	0.07
	(011)	0.12	0.03	0.95	0.03	1.02	0.08	0.16
	(010)	0.04	0.05	0.65	0.05	0.46	0.04	0.05
	(100)	0.13	0.09	1.22	0.04	1.25	0.09	0.26
	(111)	0.07	0.07	0.42	0.04	0.53	0.04	0.08
	(110)	0.06	0.01	0.08	0.03	0.11	0.01	0.05
	(101)	0.10	0.07	0.14	0.07	0.92	0.06	0.14

Table 2. Goodness of atomic fit between unreconstructed faces of hematite and ammonium sulfate (AS). Table entries are the unitless strain energies associated with atomic translation for matching between the positions of sulfate moieties and surficial iron atoms.

Supporting Information

		Corundum Face						
		(001)	(010)	(011)	(100)	(111)	(110)	(101)
AS Face	(001)	0.04	0.05	0.29	0.05	0.34	0.07	0.08
	(011)	0.08	0.02	0.48	0.06	0.68	0.13	0.16
	(010)	0.11	0.02	0.56	0.11	0.45	0.05	0.10
	(100)	0.07	0.03	0.40	0.03	0.46	0.14	0.15
	(111)	0.09	0.08	0.62	0.08	0.75	0.07	0.12
	(110)	0.10	0.05	0.31	0.03	0.68	0.06	0.15
	(101)	0.27	0.18	0.48	0.22	0.58	0.29	0.40

Table 3. Goodness of atomic fit between unreconstructed faces of corundum and ammonium sulfate (AS). Table entries are the unitless strain energies associated with atomic translation for matching between the positions of sulfate moieties and surficial aluminum atoms.

Supporting Information

		Baddeleyite Face						
		(001)	(010)	(011)	(100)	(111)	(110)	(101)
AS Face	(001)	0.09	0.08	0.04	0.02	0.12	0.05	0.12
	(011)	0.08	0.11	0.06	0.03	0.14	0.04	0.20
	(010)	0.09	0.08	0.10	0.01	0.19	0.19	0.22
	(100)	0.06	0.05	0.11	0.05	0.14	0.10	0.11
	(111)	0.16	0.13	0.17	0.08	0.23	0.27	0.28
	(110)	0.10	0.09	0.15	0.11	0.21	0.13	0.27
	(101)	0.15	0.13	0.28	0.11	0.34	0.29	0.35

Table 4. Goodness of atomic fit between unreconstructed faces of baddeleyite and ammonium sulfate (AS). Table entries are the unitless strain energies associated with atomic translation for matching between the positions of sulfate moieties and surficial zirconium atoms.

Supporting Information

		Rutile Face						
		(001)	(010)	(011)	(100)	(111)	(110)	(101)
AS Face	(001)	0.06	0.05	0.05	0.04	0.13	0.07	0.04
	(011)	0.10	0.07	0.05	0.06	0.17	0.14	0.05
	(010)	0.13	0.09	0.09	0.08	0.16	0.15	0.08
	(100)	0.07	0.08	0.06	0.03	0.20	0.25	0.08
	(111)	0.15	0.17	0.13	0.08	0.36	0.44	0.13
	(110)	0.18	0.14	0.15	0.05	0.34	0.39	0.18
	(101)	0.53	0.51	0.44	0.14	0.50	0.85	0.44

Table 5. Goodness of atomic fit between unreconstructed faces of rutile and ammonium sulfate (AS). Table entries are the unitless strain energies associated with atomic translation for matching between the positions of sulfate moieties and surficial titanium atoms.

Supporting Information

		Anatase Face						
		(001)	(010)	(011)	(100)	(111)	(110)	(101)
AS Face	(001)	0.03	0.08	0.06	0.08	0.18	0.08	0.05
	(011)	0.08	0.10	0.09	0.10	0.28	0.10	0.06
	(010)	0.01	0.06	0.09	0.12	0.33	0.14	0.06
	(100)	0.05	0.09	0.03	0.09	0.18	0.03	0.03
	(111)	0.09	0.12	0.07	0.14	0.34	0.15	0.12
	(110)	0.06	0.06	0.10	0.07	0.34	0.09	0.08
	(101)	0.08	0.15	0.09	0.19	0.42	0.08	0.04

Table 6. Goodness of atomic fit between unreconstructed faces of anatase and ammonium sulfate (AS). Table entries are the unitless strain energies associated with atomic translation for matching between the positions of sulfate moieties and surficial titanium atoms.

Supporting Information

		Mullite Face						
		(001)	(010)	(011)	(100)	(111)	(110)	(101)
AS Face	(001)	0.09	0.12	0.11	0.12	0.13	0.06	0.11
	(011)	0.13	0.22	0.22	0.01	0.22	0.05	0.22
	(010)	0.10	0.26	0.26	0.35	0.20	0.11	0.31
	(100)	0.10	0.17	0.22	0.17	0.23	0.10	0.23
	(111)	0.13	0.30	0.26	0.34	0.34	0.23	0.44
	(110)	0.14	0.34	0.27	0.32	0.37	0.30	0.39
	(101)	0.29	0.59	0.32	0.58	0.83	0.60	0.32

Table 7. Goodness of atomic fit between unreconstructed faces of mullite and ammonium sulfate (AS). Table entries are the unitless strain energies associated with atomic translation for matching between the positions of sulfate moieties and surficial aluminum or silicon atoms.