Table 1: O_2 adsorption energies at a supported Au rod on MgO as compared to unsupported Au (in parenthesis).

model	strain (%)		O_2 binding energy (eV)		
	Au	MgO	top	middle	bottom
Au rod					
along MgO[110]	+1.6	0.0	−0.45	−0.17	−0.89
			(−0.42)	(−0.06)	(−0.55)
	+0.8	−0.8	−0.04	−0.05	−0.61
			(0.04)	(−0.05)	(−0.13)
	0.0	−1.6	−0.03	−0.01	−0.44
			(−0.13)	(−0.14)	(−0.04)
Au rod					
along MgO[100]	−4.1	0.0	−0.03	−0.05	−0.19
			(0.01)	(−0.04)	(−0.01)
	−2.1	+2.1	−0.07	−0.04	0.03
			(0.06)	(−0.03)	(−0.02)
	0.0	+4.1	0.04	−0.01	−0.21
			(−0.01)	(−0.03)	(0.01)

Table 2: Adsorption energies, bond lengths, and charge of O_2 adsorbed at the interface boundary with various strain conditions; again reference values on unsupported Au are in parenthesis

model	strain (%)		$E_{O_2}^{ads}$ (eV)	d_{O-O} (Å)	charge (e)
	Au rod	MgO slab			
Au rod					
along MgO[110]	+1.6	0.0	−0.89	1.400	−0.87
			(−0.55)	(1.339)	(−0.56)
	+0.8	−0.8	−0.61	1.423	−0.94
			(−0.13)	(1.272)	(−0.27)
	0.0	−1.6	−0.44	1.403	−0.85
			(−0.04)	(1.321)	(−0.46)
Au rod					
along MgO[100]	−4.1	0.0	−0.19	1.359	−0.73
			(−0.01)	(1.272)	(−0.24)
	−2.1	+2.1	0.03	1.334	−0.66
			(−0.02)	(1.253)	(−0.13)
	0.0	+4.1	−0.21	1.337	−0.58
			(0.01)	(1.264)	(−0.18)

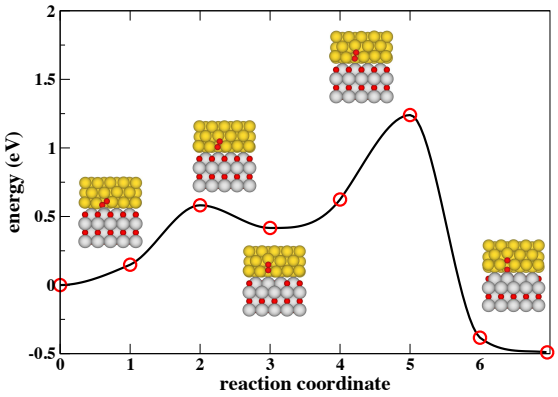

Figure 1: Minimum energy path for O_2 dissociation.

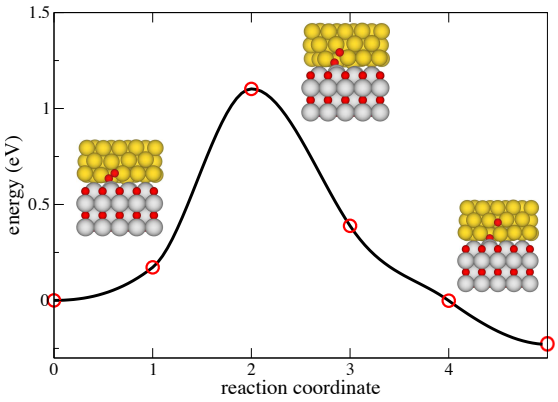

Figure 2: Minimum energy path for O_2 dissociation when an F-center is present at the Au/MgO interface.