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

Supporting Information

Al, Ga, In and Cu doped ZnO/Cu(111) bilayer films

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Table S1. Properties of CO adsorption on neighboring Zn sites of M-doped (M = Al, Ga, In and Cu) ZnO and ZnO/Cu(111) bilayer film. The CO adsorption site (Zn-T1 and Zn-T2 are denoted for the first and the second neighboring Zn sites of the top layer containing dopant, respectively, Zn-B1 and Zn-B2 are denoted for the first and the second neighboring Zn sites of the bottom layer, respectively), adsorption energy, E_{ads} (eV), magnetization, Mag (μB), Bader charge of doped metal and CO molecule, q(M/CO) (|e|), CO bond length, r(CO) (Å), metal and C (CO) distance, r(M-C) (Å), harmonic stretching frequency, ω (cm^{-1}) and the shift of frequency, $\Delta\omega$ (cm^{-1}) with respect to CO in gas phase.

System	CO site	E_{ads} (eV)	Mag (μ_B)	q(M/CO) |e|	r(CO) (Å)	r(M-C) (Å)	ω (cm^{-1})	$\Delta\omega$ (cm^{-1})
CO-Al:ZnO bilayer	Zn-T1	-0.35	0.50	2.41/-0.14	1.159	2.075	1962	-163
	Zn-T2	-0.30	0.00	2.43/-0.13	1.157	2.087	1974	-151
	Zn-B1	-0.53	-0.50	2.44/-0.22	1.164	2.050	1957	-168
	Zn-B2	-0.31	-0.50	2.41/-0.13	1.160	2.081	1956	-169
CO-Al:ZnO/Cu(111)	Zn-T1	-0.19	0.00	2.42/0.09	1.143	2.368	2120	-5
	Zn-T2	-0.29	0.00	2.43/0.08	1.141	2.240	2137	+12
CO-Ga:ZnO bilayer	Zn-T1	-0.32	0.50	1.57/-0.12	1.157	2.088	1968	-157
	Zn-T2	-0.29	0.49	1.59/-0.10	1.155	2.092	1976	-149
	Zn-B1	-0.45	0.50	1.62/-0.17	1.162	2.048	1948	-177
	Zn-B2	-0.28	0.50	1.57/-0.12	1.158	2.088	1962	-163
CO-Ga:ZnO/Cu(111)	Zn-T1	-0.18	0.00	1.63/0.02	1.144	2.406	2114	-11
	Zn-T2	-0.28	0.00	1.63/0.04	1.142	2.239	2127	+2
CO-In:ZnO bilayer	Zn-T1	0.01	0.50	1.48/-0.07	1.152	2.105	2000	-125
	Zn-T2	-0.21	1.00	0.83/0.03	1.143	2.262	2117	-8
	Zn-B1	-0.02	0.50	1.44/-0.12	1.157	2.092	1973	-152
	Zn-B2	-0.21	1.00	0.80/0.05	1.142	2.261	2132	7
CO-In:ZnO/Cu(111)	Zn-T1	-0.24	0.00	1.52/0.00	1.145	2.538	2106	-19
	Zn-T2	-0.33	0.00	1.48/0.04	1.141	2.250	2133	+8
CO-Cu:ZnO bilayer	Zn-T1	-0.19	1.00	0.97/0.03	1.143	2.273	2125	0
	Zn-T2	-0.24	1.00	0.96/0.05	1.141	2.240	2137	12
	Zn-B1	-0.23	1.00	0.92/0.03	1.142	2.280	2127	2
	Zn-B2	-0.24	1.00	0.97/0.05	1.141	2.259	2132	7
CO-Cu:ZnO/Cu(111)	Zn-T1	-0.18	0.00	0.75/-0.01	1.145	2.448	2102	-23
	Zn-T2	-0.20	0.00	0.67/0.04	1.142	2.230	2124	-1