Supporting Information for:

Impact of Electrode Potential and Solvent on the Electroreduction of CO_2: A Comparison of Theoretical Approaches

Stephan N. Steinmann[1], Carine Michel[1,2] and Philippe Sautet[1,2*]
[1]Ecole Normale Superieure de Lyon, France
[2]CNRS, France
* Corresponding author: philippe.sautet@ens-lyon.fr

To be published in: *Physical Chemistry Chemical Physics*

This supporting information was prepared on January 30, 2015 and contains 1 page.

Table 1. Net charges on the slab and Bader charges on the adsorbate and, if applicable, on the oxygen atom (Bader(O)), for selected systems for some potentials. Potentials (U) are reported in Volts with respect to the standard hydrogen electrode (SHE) and charges are in units of the elementary charge.

	Vacuum				Implicit DMF			
	U	Net-charge	Bader	Bader(O)	U	Net-charge	Bader	Bader(O)
Ni(111)	2.76	0.09			1.45	0.18		
	0.60	**0.00**			1.04	0.09		
	-1.39	-0.09			**0.58**	**0.00**		
	-3.61	-0.18			0.09	-0.09		
					-0.46	-0.18		
					-1.02	-0.26		
Na^+@ Ni(111)	1.70	0.18	0.80		-0.52	0.53	0.92	
	-0.11	0.09	0.77		-1.04	0.35	0.89	
	-1.91	**0.00**	**0.74**		-1.75	0.18	0.86	
	-3.68	-0.09	0.72		**-2.59**	**0.00**	**0.83**	
CO_2@ Ni(111)	3.52	0.09	-0.37		**1.39**	**0.00**	**-0.50**	
	1.65	**0.00**	**-0.48**		0.56	-0.18	-0.60	
	-0.23	-0.09	-0.54		-0.36	-0.35	-0.69	
	-2.07	-0.18	-0.59		-1.22	-0.53	-0.78	
	-3.91	-0.26	-0.48		-2.35	-0.70	-0.86	
CO_2,Na^+@ Ni(111)	1.16	0.09	-0.78		-0.47	0.26	-0.79	
	-0.53	**0.00**	**-0.82**		-0.94	0.09	-0.84	
	-2.18	-0.09	-0.85		**-1.27**	**0.00**	**-0.87**	
					-1.58	-0.09	-0.90	
					-1.96	-0.18	-0.93	
CO,O@ Ni(111)	**1.57**	**0.00**	**-1.19**	-0.81	**1.37**	**0.00**	**-1.16**	-0.79
	-0.43	-0.09	-1.19	-0.80	0.41	-0.18	-1.23	-0.82
	-2.44	-0.18	-1.23	-0.82	-0.63	-0.35	-1.32	-0.84
					-1.71	-0.53	-1.42	-0.88
CO,O, Na^+@ Ni(111)	2.12	0.18	-1.55	-0.98	-0.80	0.26	-1.52	-0.95
	0.30	0.09	-1.56	-0.96	-1.14	0.18	-1.55	-0.97
	-1.29	**0.00**	**-1.58**	-0.95	-1.42	0.09	-1.59	-0.98
					-1.80	**0.00**	**-1.60**	-0.96