Design and catalytic performance investigation of Ni-N-C catalyst for CO_2RR: A theoretical study

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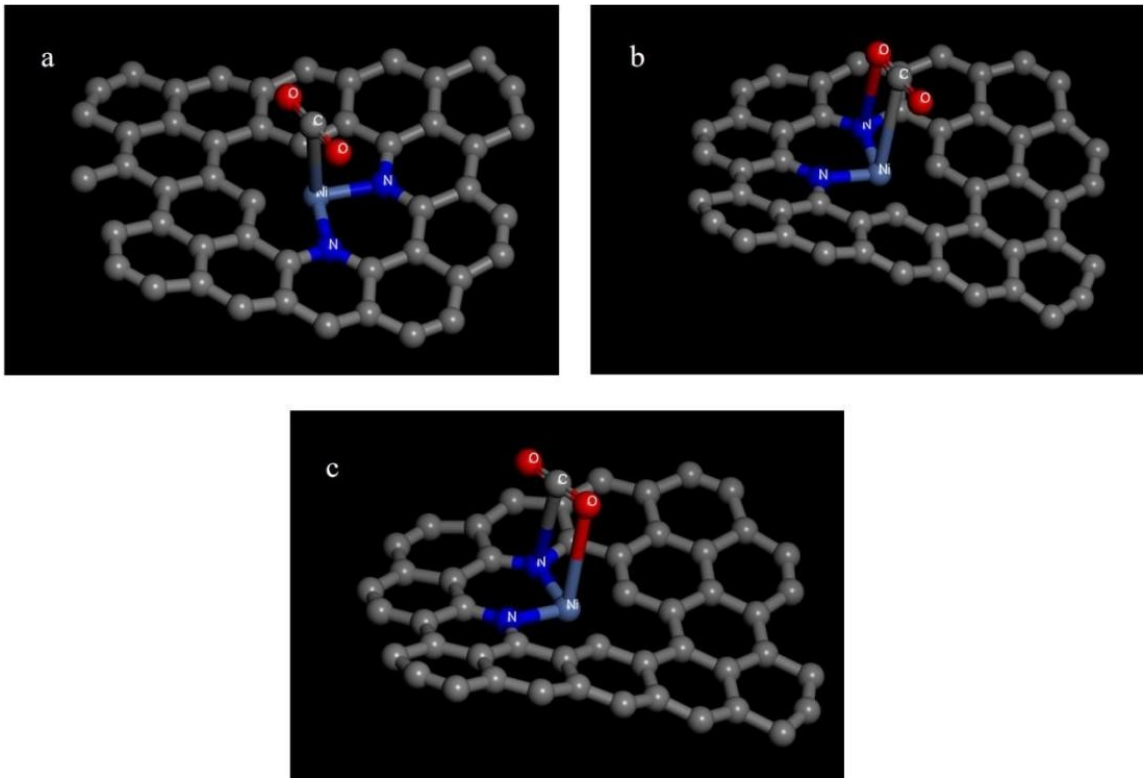

Figure S1 Isomers of the Ni-pyridine N_2V_1-C-CO_2 intermediate (a) Ni-pyridine N_2V_1-C-CO_2 single-site adsorption；(b) Ni-pyridine N_2V_1-C-CO_2 Ni-C N-O double-site adsorption；(c) Ni-pyridine N_2V_1-C-CO_2 Ni-O N-C double-site adsorption

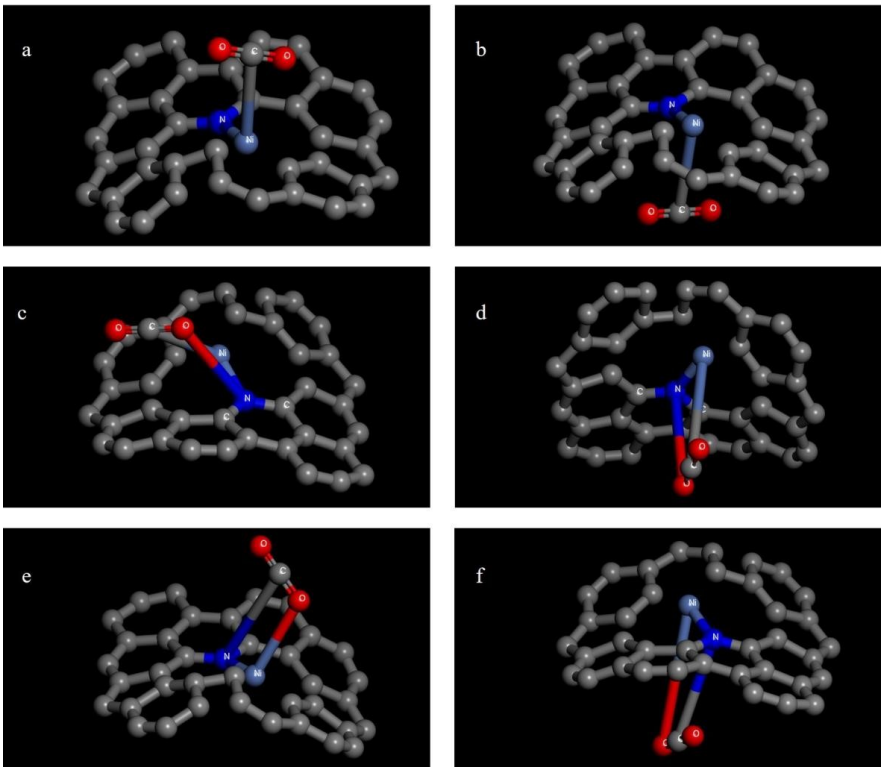

Figure S2 Isomers of the Ni-pyridine N_1V_3-C-CO_2 intermediate

(a) Ni-pyridineN_1V_3-C-CO_2 single-site adsorption A; (b) Ni-pyridineN_1V_3-C-CO_2 single-site adsorption B; (c) Ni-pyridine N_1V_3-C-CO_2 Ni-C N-O double-site adsorption A; (d) Ni-pyridine N_1V_3-C-CO_2 Ni-C N-O double-site adsorption B; (e) Ni-pyridine N_1V_3-C-CO_2 Ni-O N-C double-site adsorption A; (f) Ni-pyridine N_1V_3-C-CO_2 Ni-O N-C double-site adsorption B

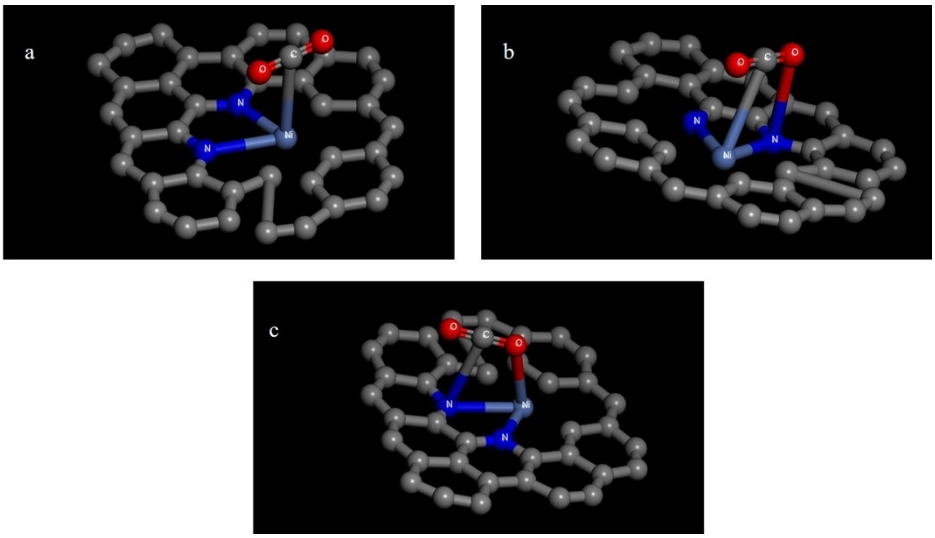

Figure S3 Isomers of the Ni-pyrrole N_1V_3-C-CO_2 intermediate

(a) Ni-pyrrole N_1V_3-C-CO_2 single-site adsorption；(b) Ni-pyrrole N_1V_3-C-CO_2 Ni-C N-O double-site adsorption；(c) Ni-pyrrole N_1V_3-C-CO_2 Ni-O N-C double-site adsorption

Table S1 Fukui index for Ni-N-C catalysts

		f(+)			f(-)	
	Atom	Mulliken	Hirshfeld	Atom	Mulliken	Hirshfeld
Ni-pyridine N_2C_1-C Catalyst Ni-C N-O	C (1)	0.012	0.014	C (1)	0.012	0.014
	C (2)	0.013	0.013	C (2)	0.013	0.013
	C (3)	0.015	0.013	C (3)	0.015	0.013
	C (4)	0.013	0.013	C (4)	0.013	0.013
	C (5)	0.013	0.013	C (5)	0.013	0.013
	C (6)	0.013	0.013	C (6)	0.013	0.013
	C (7)	0.015	0.015	C (7)	0.015	0.015
	C (8)	0.014	0.013	C (8)	0.014	0.013
	C (9)	0.01	0.011	C (9)	0.011	0.011
	C (10)	0.013	0.013	C (10)	0.013	0.013
	C (11)	0.013	0.012	C (11)	0.014	0.012
	C (12)	0.014	0.013	C (12)	0.014	0.013
	C (13)	0.013	0.012	C (13)	0.013	0.012
	C (14)	0.013	0.013	C (14)	0.013	0.013
	C (15)	0.015	0.015	C (15)	0.016	0.015
	C (16)	0.013	0.013	C (16)	0.013	0.013
	C (17)	0.012	0.013	C (17)	0.012	0.013
	C (18)	0.013	0.013	C (18)	0.013	0.013
	C (19)	0.015	0.013	C (19)	0.015	0.013
	C (20)	0.014	0.015	C (20)	0.014	0.015
	C (21)	0.015	0.016	C (21)	0.016	0.016
	C (22)	0.016	0.014	C (22)	0.015	0.014
	C (23)	0.013	0.013	C (23)	0.013	0.013
	C (24)	0.014	0.012	C (24)	0.014	0.012
	C (25)	0.014	0.013	C (25)	0.014	0.013
	C (26)	0.021	0.016	C (26)	0.02	0.016
	C (27)	0.014	0.014	C (27)	0.014	0.014
	N (28)	0.004	0.015	N (28)	0.005	0.015
	C (29)	0.013	0.013	C (29)	0.013	0.013
	C (30)	0.019	0.017	C (30)	0.018	0.017
	C (31)	0.015	0.015	C (31)	0.015	0.015
	C (32)	0.024	0.025	C (32)	0.025	0.025
	C (33)	0.014	0.013	C (33)	0.014	0.013
	C (34)	0.016	0.016	C (34)	0.016	0.016
	C (35)	0.015	0.015	C (35)	0.015	0.015
	C (36)	0.016	0.013	C (36)	0.016	0.013
	C (37)	0.015	0.015	C (37)	0.015	0.015
	C (38)	0.015	0.014	C (38)	0.015	0.014

Continued Table S1 Fukui index for Ni-N-C catalysts

		f(+)			f(-)	
	Atom	Mulliken	Hirshfeld	Atom	Mulliken	Hirshfeld
Ni-pyridine N_2C_1-C Catalyst Ni-C N-O	C (39)	0.013	0.013	C (39)	0.013	0.013
	C (40)	0.015	0.015	C (40)	0.015	0.015
	C (41)	0.014	0.014	C (41)	0.014	0.014
	C (42)	0.014	0.015	C (42)	0.014	0.015
	C (43)	0.016	0.015	C (43)	0.017	0.015
	C (44)	0.019	0.017	C (44)	0.019	0.017
	C (45)	0.019	0.014	C (45)	0.018	0.014
	C (39)	0.013	0.013	C (39)	0.013	0.013
	C (40)	0.015	0.015	C (40)	0.015	0.015
	C (41)	0.014	0.014	C (41)	0.014	0.014
	C (42)	0.014	0.015	C (42)	0.014	0.015
	C (43)	0.016	0.015	C (43)	0.017	0.015
	C (44)	0.019	0.017	C (44)	0.019	0.017
	C (45)	0.019	0.014	C (45)	0.018	0.014
	C (46)	0.015	0.013	C (46)	0.014	0.013
	C (47)	0.022	0.022	C (47)	0.023	0.022
	C (48)	0.013	0.012	C (48)	0.013	0.011
	Ni(49)	0.026	0.042	Ni(49)	0.02	0.039
	C (50)	0.012	0.011	C (50)	0.011	0.011
	N (51)	0.012	0.019	N (51)	0.012	0.019
	C (52)	0.012	0.01	C (52)	0.012	0.01
	C (53)	0.014	0.014	C (53)	0.014	0.013
	C (54)	0.014	0.014	C (54)	0.014	0.014
	C (55)	0.016	0.02	C (55)	0.017	0.02
	C (56)	0.018	0.017	C (56)	0.019	0.017
	C (57)	0.014	0.013	C (57)	0.014	0.013
	C (58)	0.012	0.013	C (58)	0.012	0.013
	C (59)	0.017	0.015	C (59)	0.017	0.015
	C (60)	0.021	0.023	C (60)	0.023	0.023
	C (61)	0.023	0.022	C (61)	0.022	0.021
	O (62)	0.041	0.037	O (62)	0.041	0.039
	O (63)	0.047	0.043	O (63)	0.047	0.045
	C (50)	0.012	0.011	C (50)	0.011	0.011
	N (51)	0.012	0.019	N (51)	0.012	0.019

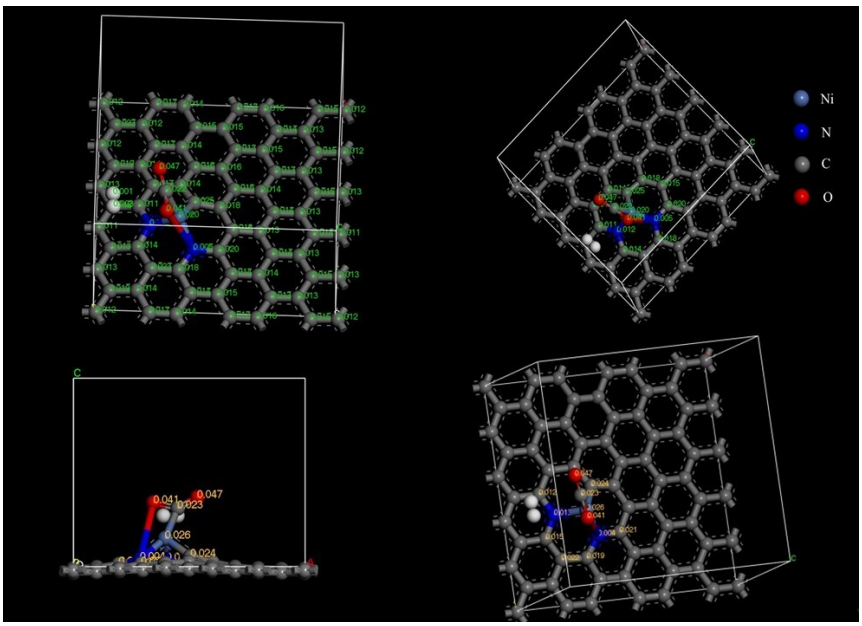

Figure S4 Fukui of Ni-pyridine N_2C_1-C Catalyst Ni-C N-O

Table S2 Adsorption energies

Catalyst		E_{ads}/ eV
Ni-pyridine N_2C_1-C	A	-0.0171
	B	-0.0088
Ni-pyridine N_1V_3-C	A	-0.0084
	B	-0.0008
Ni-pyrrole N_2V_2-C		-0.0096
Ni-pyridine N_2C_1	A	-0.0204
Ni-C N-O	B	-0.0089
Ni-pyridine N_2C_1	A	-0.0198
Ni-O N-C	B	-0.0085
Ni-pyridine N_1V_3 Ni-C N-O	A	-0.0093