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

Supporting Information

Pyridine Derivatives/Graphene Nanoribbon Composites as Molecularly Tunable Heterogeneous Electrocatalysts for Oxygen Reduction Reaction

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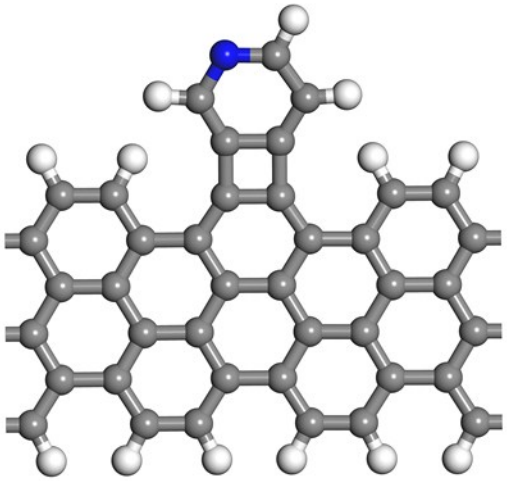
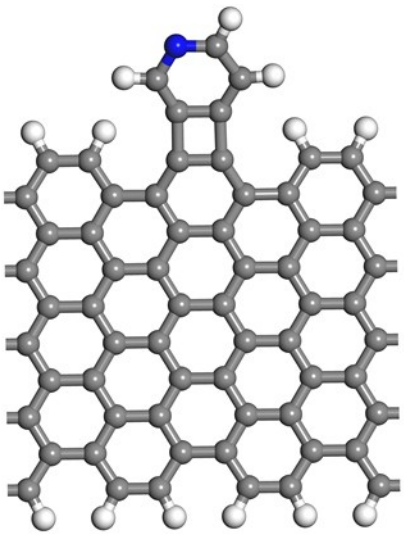
Table S1. Computed adsorption energies of ORR species on pyridine-functionalized graphene nanoribbon with models.

	E_{ads}(OOH)	E_{ads}(O)	E_{ads}(OH)
small model	-0.33	-3.92	-1.64
larger model	-0.33	-3.95	-1.66



small model



large model

Table S2. Computed adsorption energies of ORR species on pyridine-functionalized graphene nanoribbon by employing different *k* points.

	E_{ads}(OOH)	E_{ads}(O)	E_{ads}(OH)
1 × 1 × 5	-0.33	-3.92	-1.64
1 × 1 × 6	-0.32	-3.90	-1.64
1 × 1 × 7	-0.32	-3.90	-1.64
1 × 1 × 8	-0.31	-3.89	-1.64

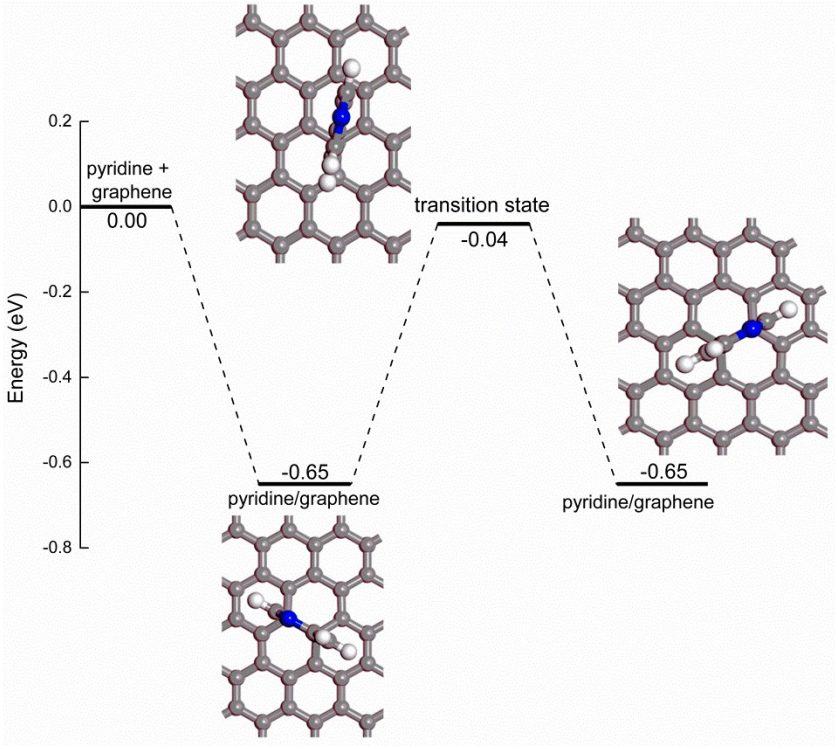


Fig. S1. The diffusion pathway of the adsorbed pyridine on pristine graphene.

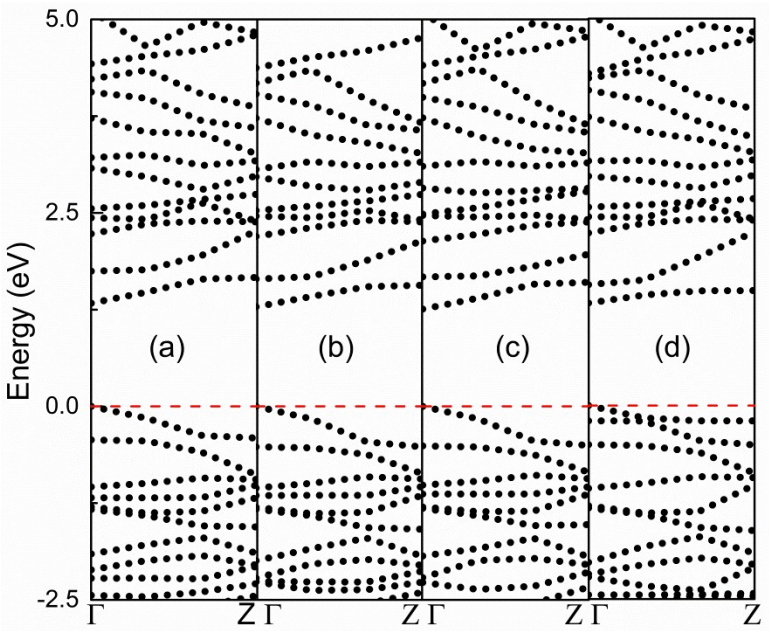


Fig. S2. The computed band structures of (a) pyridine, (b) pyridazine, (c) pyrimidine, and (d) pyrazine on the edge sites of graphene nanoribbon.