

Supporting Information

Theoretical insight into the essential role of charged surface for ammonia synthesis: Si-decorated carbon nitride electrode

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Figure S1. The Mulliken charge analysis.

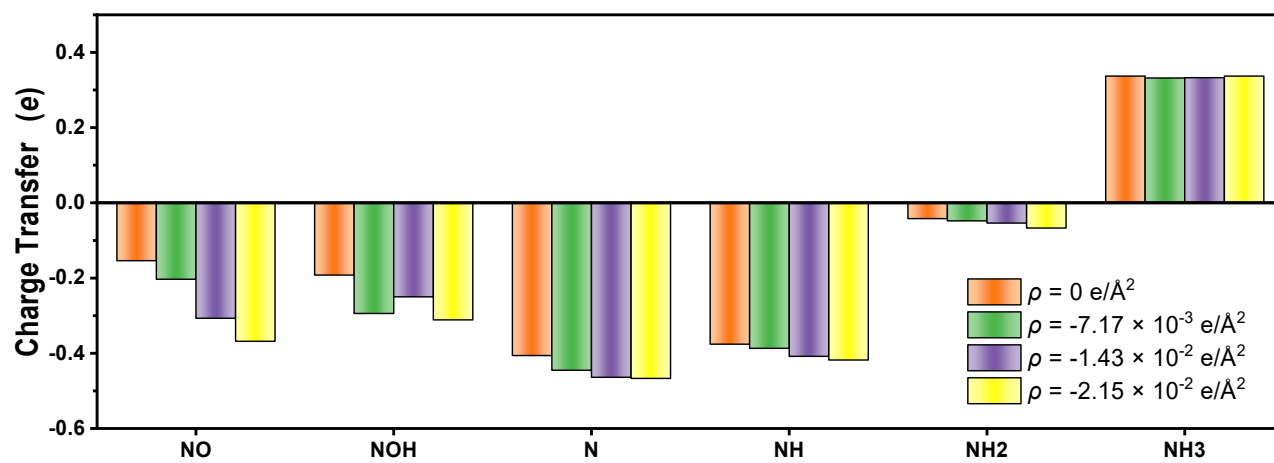


Table S1. The convergence tests for functional and k -point mesh.

	$6\times 6\times 1$	$7\times 7\times 1$	$8\times 8\times 1$	$9\times 9\times 1$
PW91	-1439.5663765	-1439.5663739	-1439.5663739	-1439.5663742
PBE	-1438.4750849	-1438.4750823	-1438.4750822	-1438.4750825
RPBE	-1440.2510039	-1440.2510009	-1440.2510011	-1440.2510014