Supporting Information

The Oxygen Reduction Reaction on Graphene from Quantum Mechanics:
Comparing Armchair and Zigzag Carbon Edges

Quang Ly, Boris V. Merinov, Hai Xiao, William A. Goddard, III, Ted H. Yu

1Department of Chemical Engineering, California State University, Long Beach, California, 1250 Bellflower Blvd, Long Beach California, 92840, USA.

2Materials and Process Simulation Center, California Institute of Technology, 1200 East California Blvd., M/C 139-74, Pasadena, California 91125, USA

Optimized initial, transition, and final image geometries (in Angstrom) for all NEB barrier calculations.

LH Mechanism – Armchair (Reaction 15 – 21)

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**LH Mechanism – Zigzag (Reaction 15-21)**

1) **OO dissociation**

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ER Mechanism – Armchair (Table VI)

OO + HOH + e⁻ → OOH + OH⁻

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\[ \text{OOH} + \text{HOH} + e^- \rightarrow \text{O} + \text{HOH} + \text{OH}^- \]

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