

Abstract Submitted  
for the MAR07 Meeting of  
The American Physical Society

**Mechanism of growth of a graphitic edge in a Carbon Monoxide atmosphere** SUJATA PAUL, ERIK E. SANTISO, MARCO B. NARDELLI, NC State University, Raleigh, NC — The interaction of CO with zigzag and armchair graphite edge has been studied using density functional theory. Our results suggest that the growth of a zig-zag graphene edge in a CO atmosphere may happen through a multiple steps. A possible growth mechanism will start through the formation of pentagon with the adsorption of CO on the edge. The cleaning of oxygen atoms from the edge could happen through the desorption of O<sub>2</sub> or desorption of CO<sub>2</sub>. Further chemisorption of CO will cover the edge with the formation of 5-7-5 structures. Such adsorptions of CO will be followed by desorption of O<sub>2</sub> or desorption of CO<sub>2</sub> and finally through the rearrangement of the 5-7-5 structures, the zig-zag edge would be restored. On the contrary the growth of armchair graphite edge have only two steps. The formation of hexagonal structures upon adsorption of CO and desorption of top oxygen atoms as CO<sub>2</sub> or O<sub>2</sub>. Our results of energy calculations suggest that the growth in the direction of a armchair wall is more favorable.

Sujata Paul  
NC State University, Raleigh, NC

Date submitted: 17 Nov 2006

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