Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Oxygen plasma etching of graphene: A first-principles dynamical inspection of the reaction mechanisms and related activation barriers[1]
KENICHI KOIZUMI, The University of Tokyo, MAURO BOERO, University of Strasbourg and CNRS, YASUTERU SHIGETA, Osaka University, ATSUSHI OSHIYAMA, The University of Tokyo, DEPT. OF APPLIED PHYSICS TEAM[2], INSTITUTE OF PHYSICS AND CHEMISTRY OF STRASBOURG (IPCMS) COLLABORATION, DEPARTMENT OF MATERIALS ENGINEERING SCIENCE COLLABORATION[3] — Oxygen plasma etching is a crucial step in the fabrication of electronic circuits and has recently received a renovated interest in view of the realization of carbon-based nanodevices. In an attempt at unraveling the atomic-scale details and to provide guidelines for the control of the etching processes mechanisms, we inspected the possible reaction pathways via reactive first principles simulations. These processes involve breaking and formation of several chemical bonds and are characterized by different free-energy barriers. Free-energy sampling techniques (metadynamics and blue moon), used to enhance the standard Car-Parrinello molecular dynamics, provide us a detailed microscopic picture of the etching of graphene surfaces and a comprehensive scenario of the activation barriers involved in the various steps.

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Date submitted: 06 Nov 2012 Electronic form version 1.4