Abstract Submitted
for the GEC14 Meeting of
The American Physical Society

Development of Ultra-Accelerated Quantum Chemical Molecular Dynamics Method for Gaseous Electronics Applications AKIRA MIYAMOTO, KENJI INABA, RYUJI MIURA, AI SUZUKI, NOZOMU HATAKEYAMA, Tohoku University, MASAAKI MATSUKUMA, KAZUYOSHI MATSUZAKI, Tokyo Electron Limited, TOHOKU UNIVERSITY COLLABORATION, TOKYO ELECTRON LIMITED COLLABORATION — Much attention has been given to the computational design of complex chemical dynamic processes including various solid surface reactions including gaseous electronics. For this purpose we have developed novel quantum chemical molecular dynamics method called ultra-accelerated quantum-chemical molecular dynamics (UA-QCMD) method which is around 10,000,000 times faster than the conventional first principles molecular dynamics method. In the present study we demonstrated that the quantum chemical calculation in UA-QCMD, that is Colors, has high accuracy in comparison with DFT and thermodynamic data. On the basis of high speed and high accuracy calculation of the UA-QCMD method we have confirmed that the method is effective for investigating dynamic mechanism of a variety of gaseous electronics processes including oxidation process of Si crystal with O_2, H_2O and O radical, oxidation process of Ge crystal with O radical and planarization process of Ru with the gas cluster ion beam (GCIB). The calculated results have been demonstrated to agree well with experimental results and give detailed mechanism of these gaseous electronics reaction processes.

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Date submitted: 11 Jun 2014 Electronic form version 1.4