Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

First principle investigations of the dielectric properties of Si3N4 thin films[1] TUAN ANH PHAM, TIANSHU LI, Department of Chemistry, University of California Davis, SADASIVAN SHANKAR, Intel Corporation, Santa Clara, California, USA, FRANCOIS GYGI, Department of Applied Science and Department of Computer Science, University of California Davis, GIULIA GALLI, Department of Chemistry and Department of Physics, University of California Davis — We have investigated the dielectric properties of silicon nitride thin films with thickness below 10 nm, by using first-principles density functional theory calculations. We find a substantial decrease of the static dielectric constant as the size is reduced, and the variation of the response in proximity of the film surfaces play a key role in the observed decrease. In addition, amorphization of the films can bring further reduction of both the static and optical dielectric constants.

[1]We acknowledge financial support from Intel Corporation

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Date submitted: 20 Nov 2009 Electronic form version 1.4