Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Transition Metal Defects in Cubic and Hexagonal Polytypes of SiC: Site Selection and Electronic Structure from ab-initio Calculations[1] ADAM GALI, VIKTOR IVÁDY, Hungarian Academy of Sciences, ANDREAS GÄLLSTRÖM, NGUYEN SON, ERIK JANZÉN, Linköping University — Relatively little is known about point defects in different polytypes of a crystal. Silicon carbide is a prototype material for polytypism. There are unidentified photoluminescence centers in SiC that are presumably originated from transition metal defects, however, the number of detected centers does not follow the number of inequivalent substitutional sites in different polytypes. In this study we applied highly convergent and sophisticated density functional theory (DFT) based methods to investigate important transition metal impurities including titanium (Ti), vanadium (V), niobium (Nb), chromium (Cr), molybdenum (Mo) and tungsten (W) in cubic 3C and hexagonal 4H and 6H polytypes of SiC. We applied DFT with PBE functional in order to calculate the ground state of the defects. We calculated the electronic structure by a screened hybrid density functional (HSE06) which was very successful in the quantitative description of native defects in SiC. We found a special asymmetric split-vacancy configuration for a class of transition metal defects. The asymmetric split-vacancy configuration exclusively prefers the hexagonal-hexagonal sites in hexagonal polytypes, thus the probability of finding these defects in 3C polytype is much smaller than in hexagonal polytypes.

[1]Swedish Foundation for Strategic Research, Swedish Research Council, Swedish Energy Agency, Swedish National Infrastructure for Computing Grants No. SNIC 011/04-8 and No. SNIC001- 10-223, Knut and Alice Wallenberg Foundation

Date submitted: 07 Dec 2011 Electronic form version 1.4