

Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Ab initio study of the adsorption, diffusion, and intercalation of alkali metal atoms on the (0001) surface of the topological insulator Bi₂Se₃ MIKHAIL OTROKOV, Donostia International Physics Center, San Sebastian, Spain, ANASTASIA RYABISHCHENKOVA, Tomsk State University, Tomsk, Russia, MIGUEL ANGEL GOSALVEZ, Donostia International Physics Center, San Sebastian, Spain, VLADIMIR KUZNETSOV, Tomsk State University, Tomsk, Russia, EVGUENI CHULKOV, Donostia International Physics Center, San Sebastian, Spain — We present the results of an *ab initio* study of the adsorption, diffusion, and intercalation of alkali metal adatoms on the (0001) stepped surface of the topological insulator Bi₂Se₃ for the case of low coverage. The calculations of the activation energies of the adatoms diffusion on the surface and in the van der Waals gaps near the steps, as well as the estimation of diffusion lengths, show that efficient intercalation through the steps is possible only for Li and Na. Data obtained for K, Rb, and Cs atoms indicate that their thermal desorption at high temperatures can start before intercalation. These results are discussed in the context of the experimental data available [?, ?].

References

- [1] Z.-H. Zhu, et al. Phys. Rev. Lett. **107**, 186405 (2011).
- [2] M. Bianchi, et al. ACS Nano **6**, 7009 (2012).

Mikhail Otrokov
Donostia International Physics Center, San Sebastian, Spain

Date submitted: 05 Nov 2015

Electronic form version 1.4