# Poster Session Program

## Bulk Fermi Surfaces of the Dirac Type-II Semimetallic Candidates $MAl_3$ (where M = V, Nb and Ta)

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**Abstract**

We report a de Haas-van Alphen (dHvA) effect study on the Dirac type-II semimetallic candidates MAl3 (where, M = V, Nb and Ta). The angular-dependence of their Fermi surface (FS) crosssectional areas reveals a remarkably good agreement with first-principle calculations. Therefore, dHvA supports the existence of tilted Dirac cones with Dirac type-II nodes located at 100, 230 and 250 meV above the Fermi level $E_f$ for VAl3, NbAl3 and TaAl3 respectively, in agreement with the prediction of broken Lorentz invariance in these compounds. However, for all three compounds we find that the cyclotron orbits on their FSs, including an orbit nearly enclosing the Dirac type-II node, yield trivial Berry phases. We explain this via an analysis of the Berry phase where the position of this orbit, relative to the Dirac node, is adjusted within the error implied by the small disagreement between our calculations and the experiments.

## Lithium Intercalation in Graphene/MoS Heterobilayers

Daniel T. Larson, Ioanna Fampiou, Gunn Kim, Efthimios Kaxiras

**Abstract**

Abstract: Two dimensional (2D) heterostructures have attracted great scientific interest as candidate materials for highly efficient energy storage devices due to their potential for high carrier capacity via reversible ionic intercalation. In this study we employ density functional theory calculations to investigate the structural and electronic properties of lithium-intercalated Graphene/Molybdenum Disulfide (Gr/MoS) heterostructures, and the extent to which Li intercalates at the interface formed between graphene (Gr) and molybdenum disulfide (MoS) layers. We explore in detail the adsorption and diffusion of Li atoms, the energetic stability and changes in the structural morphology of MoS from the 2H to 1T' phases, and the corresponding electronic structure and charge distribution within the heterostructure with varying concentrations of Li. Our results indicate that the maximum energetically allowed ratio of Li to Mo (Li to C) is 1:1 (1:3) for both MoS polymorphs. This is double the Li concentration allowed in graphene bilayers, as shown in previous work. We find that there is 60% more

charge transfer to MoS than Gr in the bilayer heterostructure, which results in a maximum doping of Gr and MoS equal to and , respectively. Our results provide a framework for understanding Li intercalation in experimentally fabricated Gr/MoS structures and encourage tailored design of 2D energy storage devices through variation of intercalant concentration and layer polymorphs.

# Enhanced magnetism and improved anisotropy in $Ce_2Co_{17}$ via Sm substitution at $Ce_{2c}$ site

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**Abstract**

The magnetocrystalline anisotropic energy (MAE) of hexagonal $Ce_2Co_{17}$ is very low and can't be useful for permanent magnets. We have tried to improve anisotropy via site selective 2c-substitutional doping of Ce by Sm. The present calculations of the electronic and magnetic properties of $Ce_2Co_{17}$ and $SmCeCo_{17}$ have been performed using the full potential linear augmented plane wave (FPLAPW) method within the generalized gradient approximation (GGA). For Sm-substitution, Coulomb correction in GGA (i.e. GGA+U) has been added to provide better representation of energy bands due to the strongly correlated Sm-atoms. The Sm-substitution at $Ce_{2c}$ sites favors incremental uniaxial MAE. These trends so observed in the MAE for this substitution have been examined in terms of contributions from various electronic states. Finally, $SmCeCo_{17}$ have been predicted as potential material for designing permanent magnets based on saturation magnetism and MAE observed.

# Fermi surface study of the type-II Weyl semimetal candidates $WP_2$ and $MoTe_2$

Rico U. Schoenemann

**Abstract**

Weyl type-II fermions are massless quasiparticles that obey the Weyl equation and which are predicted to occur at the boundary between electron and hole pockets in certain semimetals, i.e. the (W,Mo)(Te2,P2) compounds. Here, I present a study of the Fermi surface of WP2 via measurements of the Shubnikov-de Haas (SdH) e_ect. Compared to other semimetals, WP2 exhibits a very low residual resistivity, i.e., _ = 10 ncm, which leads to perhaps the largest nonsaturating magnetoresistivity reported for any compound. The angular dependence of the SdH frequencies is found to be in excellent agreement with the _rst-principles calculations when the electron and hole bands are shifted by 30 meV with respect to the Fermi level. Additionally the results are compared with a previous study on orthorhomic MoTe2 where signi_cant di_erences between the experimental results from de Haas-van Alphen oscillations and DFT calculations have been found - thus questioning the existence of Weyl points in this material.

# Thermoelectric properties of monoclinic NaSbSe2

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**Abstract**

We explore the thermoelectric properties of NaSbSe2 using first principles and transport calculations. Previously known to exist in its disordered rock-salt type structure which has too low band gap for thermoelectric applications, its stable nanocrystalline (layered) monoclinic form with suitable band gap was synthesized recently. Our calculation suggests a favorable combination of conductivity and thermopower. The iso-energy surface plots have certain degree of anisotropy reflected in the electrical conductivity arising from the layered structure. The electron fitness function supports the results indicating good thermoelectric properties at par with the currently best known thermoelectric materials, especially for the n-doped system.