On behalf of the

Science College CMS
Vienna Computational Materials Laboratory
and Center for Computational Materials Science

we cordially invite you to the following seminar

Dr. Aleksey N. Kolmogorov

Department of Materials, University of Oxford

Search for new synthesizable materials with ab initio methods

Screening large configurational spaces of structures and compositions for new synthesizable materials with desired properties poses a number of computational challenges. I will overview recent advances in the compound prediction methodology which now allows identification of complex ground states with little or no experimental input. Our recent work demonstrates the effectiveness of a combined high-throughput and evolutionary algorithm [1] approach leading to a number of unexpected

findings: we have shown that new compounds with never-seen-before structures should form in common, technologically relevant metal boride systems [1-4]. One of the proposed materials has the potential to be a phonon-mediated Fe-based superconductor with a Tc of 15-20 K [2,3] and another could be a cheap superhard material stable under ambient conditions [4].

[1] A. N. Kolmogorov, http://maise-guide.org [2] A. N. Kolmogorov, S. Shah, E. R. Margine, A. F. Bialon, T. Hammerschmidt, and R. Drautz, Phys. Rev. Lett., 105, 217003 (2010) [3] A. F. Bialon, T. Hammerschmidt, R. Drautz, S. Shah, E. R. Margine, and A. N. Kolmogorov, Appl. Phys. Lett., 98, 081901 (2011) [4] H. Niu, J. Wang, X.Q. Chen, D. Li, Y. Li, P. Lazar, R. Podloucky, and A. N. Kolmogorov, submitted (2011)

Date: Monday, Nov 07, 2011   16:00
Location: Seminar room 138C (TU Freihaus 9. Stock, <mark>gelb</mark>)
               A-1040 Wien, Wiedner Hauptstaße 8-10