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Electronic Structure with Muffin-tins**Liviu Chioncel, University of Augsburg, Germany**

Professor

Digital Media Center 1008B
May 30, 2019 - 09:30 am**Abstract:**

The Exact Muffin-tin Orbitals (EMTO) theory was developed by O.K. Andersen and collaborators starting from the 90s [1]. This method was implemented by L. Vitos [2] of KTH Stockholm and was the first to allow Dynamical Mean-Field Theory (DMFT) formulation within the multiple scattering approach [3]. With a DMFT solver formulated on the Matsubara energies, this method suffers due to the analytic continuation inserted into the iteration steps [4]. We reformulated the LDA+DMFT scheme for the EMTO basis set without the need of analytic continuation [5]. This was recently extended to include on-site disorder within the Coherent Potential Approximation, in addition to DMFT [6]. Even more recently we have succeeded to implement an ab-initio typical medium theory [7].

[1] O. K. Andersen, T. Saha-Dasgupta PRB 62, R16219 (2000)

[2] L. Vitos et. al. Comput. Matter. Sci. 18, 24 (2000)

[3] L. Chioncel et. al. PRB 67 235106 (2003)

[4] A. Oestlin, L. Chioncel, L. Vitos. PRB 86 235107 (2012)

[5] A. Oestlin, L. Vitos, L. Chioncel PRB 96 125156 (2017)

[6] A. Oestlin, L. Vitos, L. Chioncel PRB 98 235135 (2018)

[7] Augsburg, Louisiana, Stockholm collaboration

Speaker's Bio:

Liviu Chioncel studied physics in Cluj-Napoca, Romania and Grenoble, France. He received his PhD in physics from the University of Nijmegen, Netherlands in 2004 and his habilitation from the Technical University Graz, Austria in 2010. He is professor of theoretical physics at the University of Augsburg, Germany. His research covers DMFT models and ab-initio, DFT and materials science, scattering theory (Compton/positron Annihilation), Disorder (weak and strong), transport.

