West Virginia University
BENJAMIN M. STATLER COLLEGE OF ENGINEERING AND MINERAL RESOURCES

MATERIALS SCIENCE AND ENGINEERING (MS&E) SEMINAR SERIES

Friday October 16, 2020 at 3:00 pm via Zoom

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"Modeling the electronic structure of strongly correlated materials: from DFT to DMFT with some Machine Learning spices"

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Abstract: Abstract: In this talk, we will discuss the different physical approaches researchers have been using to describe strongly correlated materials (many of the materials with atoms in the d- and f- blocks of the periodic table). We will introduce these materials' potential applications and why the people are so excited about controlling their response. While density functional theory is the most used method to describe the electronic properties of materials, it fails in describing many of the interesting phenomena in this type of material. We will overcome this problem by introducing the so-called dynamical mean-field theory method, avoiding the complex mathematical discussion, and providing the theory's physical insight. We will finalize by discussing some of the research projects we are now working on in this arena and how we see the future of this research, particularly how novel methods of Machine Learning can provide some understanding of the physics in these complex systems.

Bio: Aldo Humberto Romero education consist of Universidad de los Andes, Bogota, Colombia, with a Physics, B.Sc. and a Civil Engineering, BEng, 1990. Received his Ph.D. of Physics and Chemistry at University of California-San Diego. Aldo completed his Postdoc in Physics at Max Planck Institute, Stuttgart, Germany in 1999-2000. Research and Professional Experience: At present Aldo is a Professor, Physics Department, West Virginia University.

More than 220 publications mostly on computational physics (with an average of 10 papers per year for the last 12 years) in journals such as Science, Physical Review Letters, NanoACS, Nanoletters, etc. AN H-index of 46, with more than 9000 citations. He is the author of a book on computational characterization of materials. Fellow of the American Physical Society and Member of the Mexican Academy of Science.

Main developer of the computational packages: PyProcar, DMFTvsDFT, ELK, PyElastic, PyChemia and developer of Abinit (www.abinit.org) XRAC-XSEDE-NSF Evaluation Committee, 2018-2021. Assistant editor of European Journal of Physics B and Materials. Member of the developer group of the first principle software ABINIT and Chair of the international advisory committee (www.abinit.org

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