UC San Diego
JACOBS SCHOOL OF ENGINEERING
NanoEngineering

UCSD NanoEngineering/Chemical Engineering

SPECIAL SEMINAR

Friday, March 6, 2020
Seminar Presentation: 1:30pm – 2:30pm
SME room 248

"Machine Learning meets First Principles towards a Periodic Table of Materials and Reactions"

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Abstract: Computational chemistry and materials science algorithms are now powerful enough that they can predict many properties of materials and molecules before they are synthesized. By implementing and developing new approaches to calculate materials and chemical properties in supercomputers, we have predicted over 300,000 materials for energy storage and catalysis.
The computations predicted several new materials which were made and tested in the lab. The creation of our large amount of materials in-silico, has prompted to create our own type of materials Atlas for different purposes. We have implemented different machine learning methods to find further (materials or reaction) design principles.
Some of the applications of the design principles of materials has been used towards developing an alternative way to generate and store energy; specifically, in the next generation batteries, Hydrogen (H2) and Artificial Photosynthesis.

Educational and training statement: (1) What Scientific Societies Can Do for You. There are several programs embedded in scientific societies that help you in the path of higher education. (2) applying to graduate school (app process and APS/ACS/MRS bridge program). I am part of the national committee of minorities so I can talk about the program that we have pushed early on: "The NSF INCLUDES Alliance: IGEN (Inclusive Graduate Education Network) is a partnership of over 30 societies, institutions, organizations, corporations, and national laboratories poised to lead a paradigm shift in increasing the participation of underrepresented racial and ethnic minority (UREM) students who enter graduate or doctorate level programs in the physical sciences."
http://igenetwork.org/
https://www.aps.org/publications/apsnews/201810/igen.cfm

Biosketch: Dr. Mendoza-Cortes received his BSc from UCLA and Monterrey Tech, his PhD from CalTech in 2012 with Bill Goddard and did his PDF from UC Berkeley in 2014 with Martin Head-Gordon. Dr. Mendoza-Cortes has worked in the field of Theoretical and Computational Material Sciences, Physics and Chemistry for more than 13 years. Dr. Mendoza-Cortes has pioneered concepts for Materials by Design in combination with atomistic simulations and new algorithms. The first example was published in Science magazine and was awarded the AAAS Newcomb Cleveland Prize, which is the AAAS's oldest and most prestigious award. His recent research about designing new materials for energy conversion was featured in Forbes magazine, CNBC and the Department of Energy (DOE) highlights.
His published work has 5,094 total citations or an average of around 163 citations per paper (i10-index = 20). Because of graduate and post-graduate studies advisors, Dr. Mendoza-Cortes' academic great grandparents are Marie Curie and Paul Dirac.