

THE MATERIALS SCIENCE AND ENGINEERING DEPARTMENT WINTER COLLOQUIUM SERIES PRESENTS:

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Materials by Design: First-Principles for Energy Storage.

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 100,000 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 using these materials genomes to find further materials 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, as well as to develop the first periodic table of materials (allotropes, 2D-materials, chelation for radioactive materials, earth abundant semiconductors and Porous materials).

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 have 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 experiments. 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 5,070 total citations or an average of around 163 citations per paper. Journals in which we have published include: Science, Physical Reviews, Adv. Energy Materials, Nature Comm. to name a few.

Because of graduate and post-graduate studies advisors, Dr. Mendoza-Cortes' academic great grandparents are Marie Curie and Paul Dirac. Dr. Mendoza-Cortes has changed fields several times.

Tuesday, March 10 • 4 pm | Tech L211