American Mineralogist, Volume 109, page 960, 2024

Presentation of the Dana Medal of the Mineralogical Society of America for 2023 to Razvan Caracas

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It is my great honor to present my good friend and colleague, Razvan Caracas, the recipient of the 2023 Dana Medal. The Dana Medal recognizes sustained, outstanding scientific contributions through original research in the mineralogical sciences by an individual in the midst of their career.

Razvan is a computational mineral physicist who works on an impressive range of problems ranging from the composition of the Earth's core to the dynamics of Moon formation. His work demonstrates a unique talent, creativity, and collaborative spirit to extend the results derived from the atomic-scale calculations to planet-scale processes. Razvan Caracas is an expert in ab-initio calculations, that is, calculations that are used to solve the Schrödinger Equation of a suite of electrons and their atomic cores. Unfortunately, solving the Schrödinger Equation exactly, accounting for every electron and every nucleon, is a computationally impossible problem. The science and art of these calculations is to approximate the problem without sacrificing the fundamental physics. This is at the heart of Razvan's work and where his talents shine: With each scientific contribution is a careful set of calculations grounded in their fundamental physics through these "first-principles" calculations.

For example, very shortly after the first description of the post-perovskite phase, a mineral structure proposed to be responsible for seismic transitions observed at the base of the Earth's mantle, Razvan probed the effects of more realistic chemistry on the transition. In this work, he mapped out how introducing iron and aluminum to the system affected the depth to the transition and the phase's elastic wave speeds. Both results have withstood the test of time by seismic observations and multiple subsequent experiments on this system.

More recently, with the greatly expanded computational capacity of compute clusters, Razvan has focused on the physical and chemical properties of melts that form in low-density conditions after a giant impact event such as that which formed the Moon. Recognizing that his calculations were demonstrating fracturing of the melt, Razvan was able to use elegant thermodynamics to interpret the results, mapping out the liquid-gas equilibrium point as a function of composition, as well as identify components of the system that formed in the gaseous state, which indicate components of our proto-atmosphere.

Winding its way through his scientific contributions, we see a theme in Razvan's work where he consistently shares his efforts with both the scientific community and the general public. Beginning as a Ph.D. student and extending across much of his career to date, Razvan has contributed to the development of ABINIT, a software suite to calculate observable properties of materials from first principles. More recently, he is the developer of codes and databases for the interpretation of those ab-initio results. He has also been convenor of workshops and summer schools to introduce others to the tools he's developed or contributed to. This and other code development and sharing efforts of his are critical contributions that enable scientists to perform and interpret the results of their work.

Extending his spirit of sharing his science with the wider public, the exhibition "Moon Impact, a Geological Story" tells the story of the Moon-forming Giant impact in the context of the geological evolution of the Earth and of the solar system. Time flows inside the exhibition, starting with the formation of the solar system and ending with the present day. The exhibition features geologic samples and meteorites, movies, and 3D printed models of the atoms in melts and volcanic gas bubbles stemming from atomistic simulations from Razvan's computational results. This exhibition opened first in 2021 at two sites in his native Romania before moving to Bulgaria, and now with planned visits in Germany and beyond.

Razvan's scientific productivity has been extraordinary, with more than 115 published papers. This productivity can be attributed to a number of factors. First, he possesses the ability to identify major problems that are of broad interest to solid-Earth geophysicists. Second, he is not only an extraordinarily careful and innovative computational scientist, but he also can develop sophisticated yet computationally feasible approaches and interpretation schemes. Third, he is a willing and enthusiastic collaborator, which has enabled him to develop numerous productive collaborations with scientific colleagues from all over the world.

As this year's Dana Medalist, I look forward to whatever Razvan Caracas tackles next.

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0003-004X/24/0005–960$05.00/DOI: https://doi.org/10.2138/am-2024-AP10954