Abstract Submitted
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The Age of Exploration: Materials Discovery in the Virtual World[1] KARIN RABE, Rutgers, the State University of New Jersey — New materials can solve many (though not all) of the world's problems though faster, smaller-scale and cheaper processing and storage of information and energy. Improving and optimizing the materials we already use for these purposes can only take us so far – what about something really new? How would we know where to look? Information about the structures and properties of experimentally known materials, as organized into a crystallographic database, provides the initial data for a rough map of the space of possible materials. Using the theory of quantum mechanics to perform first-principles computer simulations of the properties of known and as-yet hypothetical materials from first principles, using only their chemical composition as input, we can augment the database with the results of computer experiments to develop the map. By constructing materials models from first-principles information, we can identify the regions of the map that are the most rewarding for closer study at each stage. As the map develops, we can target relatively little-studied families of materials to identify promising candidate materials with desired properties and provide guidance to experimenters in the real world, allowing them to focus their efforts in the most productive directions; this is the underlying principle of the Materials Genome Initiative of 2011. In this talk, I will describe what functional materials are and how they work, with illustrative results including ferroelectrics, antiferroelectrics, multiferroics, and field-controlled metal insulator systems, both in bulk form and in artificial heterostructures. The challenges and promise of theoretical materials design and theoretical-experimental integration will be discussed.

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Karin Rabe
Rutgers, the State University of New Jersey

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