# Alex Zunger receives inaugural Materials Theory Award

The Materials Research Society has named Alex Zunger of the University of Colorado–Boulder to receive the inaugural Materials Theory Award for his "development of the Inverse Band Structure approach to materials by design and the foundational developments of methods of First-Principles theory of solids, leading to innovative and transformative studies of renewable-energy materials and nanostructures." Zunger will be recognized during the awards ceremony at the 2011 MRS Fall Meeting in Boston. The Materials Theory Award, endowed by Toh-Ming Lu and Gwo-Ching Wang, "recognizes exceptional advances made by materials theory to the fundamental understanding of the structure and behavior of materials."

Zunger has made seminal contributions as a theorist working in the area of condensed matter and materials physics. He made foundational contributions to the development of the pseudopotential-total energy approach to predict and explain properties of solids and to the development of exchange-and-correlation functions for computing electron–electron interactions in density functional theory. His theoretical work on semiconductor alloys, complex semiconductors, and nanostructures were contributions at the forefront of these fields.

His recent work is motivated by the goal to predict structural arrangements to design materials with desirable electronic properties. Prior to Zunger's proposal of an "inverse approach," the standard protocol was to first state the underlying *structure* of a solid or molecule (e.g., its symmetry, or structure type), then predict the system's *properties* (e.g., optical, mechanical, electric, magnetic) through quantum calculations. However, this approach did not reveal how the atomic structure should be changed to achieve a certain target property.

Zunger's idea was to *start* by articulating the material property desired for a particular technology (e.g., optical, mechanical, electric, magnetic), *and then* calculate the structure that would have the target property. For example, in his pioneering work on the design of semiconductor quantum nanostructures, he asked the question, "If you had any amount of GaAs 'planes' and AlAs 'planes,' how would you stack them (and in what direction) so that the ensuing structure has the largest possible bandgap (i.e., shortest-wavelength absorption)?" Using simulated annealing for this search and pseudopotential calculations for the electronic structure, he found that only about 10,000 band structures need to be examined (out of $10^{14}$ possibilities) to find the one that fits the target. Zunger demonstrated that simulated annealing and genetic algorithms, coupled with quantum theory, can rapidly "learn" the "landscape" and deliver an answer. The result was that a particular superstructure with layers oriented along the (201) direction produces the largest possible bandgap. His work now forms the basis for an office of science "Energy Frontier Research Center on Inverse Design," combining his theoretical work with the experimental work of groups at National Renewable Energy Laboratory (NREL), Northwestern University, Stanford SLAC National Accelerator Laboratory, and Oregon State University, who are realizing some of these target structures.

Zunger received a PhD degree from Tel Aviv University, Israel. He held postdoctoral research positions at Northwestern University and the University of California–Berkeley. At NREL, he established the Solid State Theory group where he has mentored over 70 postdoctoral fellows. He is a fellow of the American Physical Society. His honors include the John Bardeen Award of the Minerals, Metals & Materials Society, the Rahman Award of the APS, the Tomassoni Prize and Physics Medal of the Scola Romana di Physica, and the Guttenberg Award of Science.