Enhanced efficiency when determining band gap in solids

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(PhysOrg.com) -- "With density functional theory, we are able to put different elements in a computer simulation and do calculations based on quantum mechanics to find out about their different properties," Maria Chan tells *PhysOrg.com.* However, density functional theory is not entirely helpful in identifying all the properties associated with different compounds.

Chan, a post-doc at Argonne National Lab (formerly at MIT), points out that the theory is lacking when it comes to band gaps. "The band gap problem is a well known one. However, using current methods, there is quite a bit of inaccuracy when it comes to calculating band gaps." Band gaps in solids are important, especially if researchers want to identify the best materials for a variety of functions. The maximum efficiency of a solar cell, for example, is determined by the band gap of the material. "The inability to predict the band gap is holding back research in photovoltaics, as well as in semiconductors and thermoelectrics," Chan points out.

However, Chan thinks that a solution might have been found. Working with professor Gerbrand Ceder at MIT, it appears that a modified application of density functional theory – with a special generalization for solids – might hold the key to more accurate predictions of band gaps. The work is described in *Physical Review Letters*: "Efficient Band Gap Prediction for Solids."

“In the past, researchers have broken down individual electrons using a

sort of itemized list of individual states. This has allowed for calculations revealing different properties, including band gaps. Unfortunately, the accuracy of the band gap predictions has been off," Chan says. She points out that scientists know that silicon has a band gap of about 1.2 eV, but when current methods are employed to calculate the band gap, the answer is 0.7 eV. "You can see how that's a problem if you are trying to gauge the suitability of a material for specific purposes," she continues.

To get a more accurate prediction of band gaps, Chan and Ceder created a method that involves altering the use of density functional theory so that an itemized list of individualized states is not the only consideration. "We also recognize that there are a number of interactions between electrons. So we look at the total energy, which includes these interactions," Chan explains.

Not only do Chan and Ceder make use of the total energy, but they also demonstrate that the band gap can be viewed as a property of the ground state. "This changes the way we view the band gap, seeing that it is a part of the ground state," Chan says.

Moving forward, Chan hopes that this technique can be used to identify the band gaps of different materials with more accuracy. This could prove useful in identifying the best options when creating future technology. "This work is part of the Materials Genome project started by Professor Ceder, with a goal of predicting properties of known compounds and using the knowledge to design new ones," Chan says. "Part of that is understanding the band gap and being able to quickly determine the band gaps of various materials."

"Our method is relatively inexpensive, and could be useful when learning the properties of new materials," Chan continues. "If someone came up with a new kind of material, predicting the band gap is not a question

easily answered in the past. Hopefully our work will pave the way for easier answers in the future."

More information: M.K.Y. Chan and G. Ceder, "Efficient Band Gap Prediction for Solids," *Physical Review Letters* (2010). Available online: prl.aps.org/abstract/PRL/v105/i19/e196403