Researchers develop algorithm to make simulation of ultrafast processes possible

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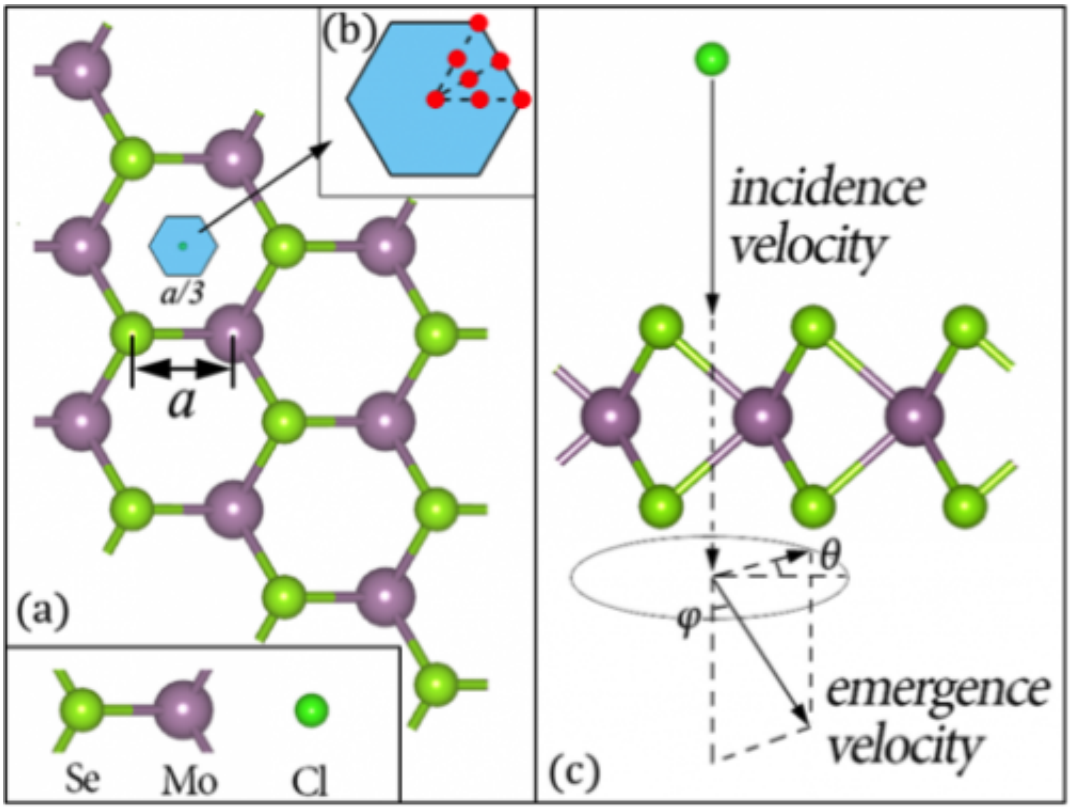


Model of ion (Cl) collision with atomically thin semiconductor (MoSe2). Collision region is shown in blue and zoomed in; red points show initial positions of Cl. The simulation calculates the energy loss of the ion based on the incident and emergent velocities of the Cl.

When electronic states in materials are excited during dynamic processes, interesting phenomena such as electrical charge transfer can

take place on quadrillionth-of-a-second, or femtosecond, timescales. Numerical simulations in real-time provide the best way to study these processes, but such simulations can be extremely expensive. For example, it can take a supercomputer several weeks to simulate a 10 femtosecond process. One reason for the high cost is that real-time simulations of ultrafast phenomena require "small time steps" to describe the movement of an electron, which takes place on the attosecond timescale – a thousand times faster than the femtosecond timescale.

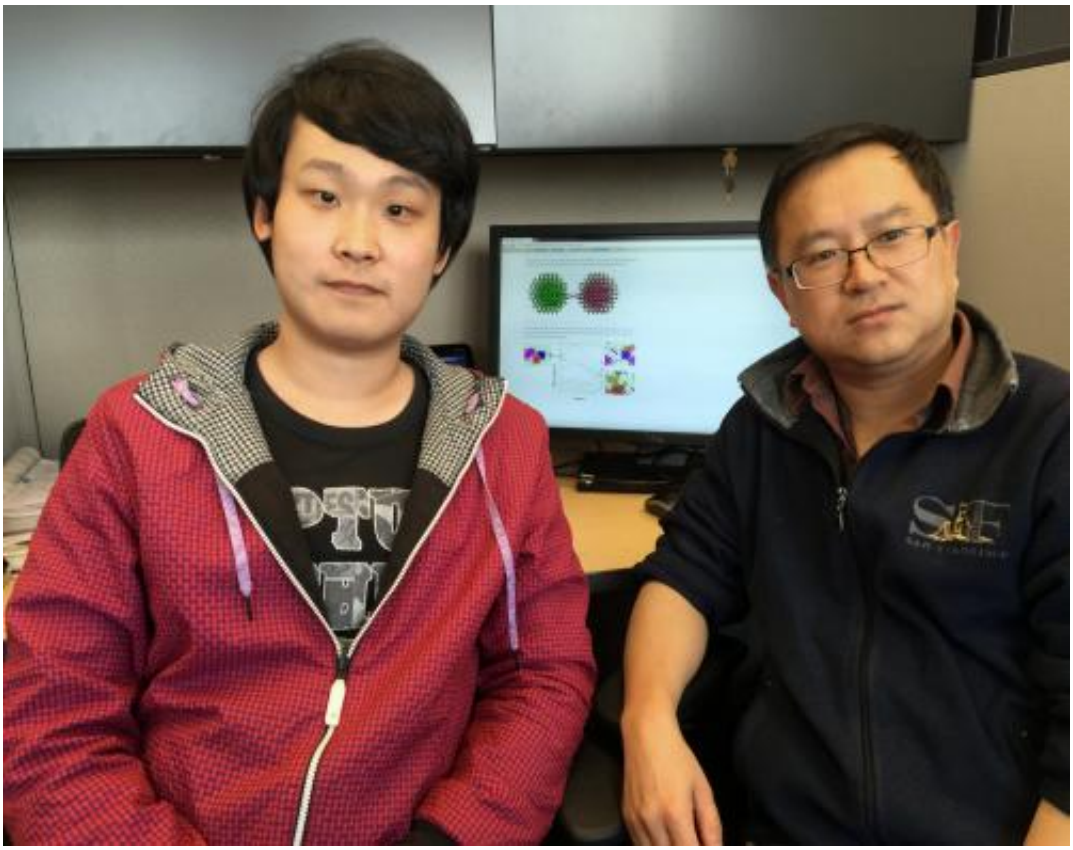
To combat the high cost associated with the small-time steps, Lin-Wang Wang, senior staff scientist at the Lawrence Berkeley National Laboratory (Berkeley Lab), and visiting scholar Zhi Wang from the Chinese Academy of Sciences, have developed a new algorithm which increases the small time step from about one attosecond to about half a femtosecond. This allows them to simulate ultrafast phenomena for systems of around 100 atoms.

"We demonstrated a collision of an ion [Cl] with a 2D material [MoSe2] for 100 femtoseconds. We used supercomputing systems for ten hours to simulate the problem – a great increase in speed," says L.W. Wang. That represents a reduction from 100,000 time steps down to only 500. The results of the study were reported in a *Physical Review Letters* paper titled "Efficient real-time time-dependent DFT method and its application to a collision of an ion with a 2D material."

Conventional computational methods cannot be used to study systems in which electrons have been excited from the ground state, as is the case for ultrafast processes involving charge transfer. But using real-time simulations, an excited system can be modeled with time-dependent quantum mechanical equations that describe the movement of electrons.

The traditional algorithms work by directly manipulating these

equations. Wang's new approach is to expand the equations into individual terms, based on which states are excited at a given time. The trick, which he has solved, is to figure out the time evolution of the individual terms. The advantage is that some terms in the expanded equations can be eliminated.



Zhi Wang (left) and Lin-Wang Wang (right)

"By eliminating higher energy terms, you significantly reduce the dimension of your problem, and you can also use a bigger time step," explains Wang, describing the key to the algorithm's success. Solving the equations in bigger timesteps reduces the computational cost and increases the speed of the simulations

Comparing the new algorithm with the old, slower algorithm yields similar results, e.g., the predicted energies and velocities of an atom passing through a layer of material are the same for both models. This new algorithm opens the door for efficient real-time simulations of ultrafast processes and electron dynamics, such as excitation in photovoltaic materials and ultrafast demagnetization following an optical excitation.

More information: "Efficient Real-Time Time-Dependent Density Functional Theory Method and its Application to a Collision of an Ion with a 2D Material." *Phys. Rev. Lett.* 114, 063004 – Published 13 February 2015. journals.aps.org/prl/abstract/ … ysRevLett.114.063004

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