Popular Summary: QED theory of electron beam-induced electronic excitation and sputtering in 2D crystals

The ability to control a material's structure atom-by-atom can provide powerful solutions to many of today's most pressing technological and environmental challenges. To this end, electron beam irradiation can be used for precise material sculpting by selectively nudging individual atoms with high-speed electrons. In this way, atomic-scale features can be chiseled into the material through a process called sputtering, in which a high-speed beam electron knocks an atom out of the material.

The theory of electron collisions with matter was first developed over 100 years ago, and has since undergone only slight modifications to account for relativistic and thermal effects. However, recent experiments have shown that modern theoretical models often drastically underestimate sputtering rates in two-dimensional (2D) insulators, a class of materials possessing enormous potential for nanotechnology. This is because the majority of current models focus solely on the interaction between the beam electron and material's nuclei, neglecting the possibility that the beam electron can also collide with and excite the material's electrons. In insulators, these electronic excitations can weaken the bonding between the irradiated atoms, increasing their sputtering rates.

To account for this phenomenon, we have developed a first-principles method to calculate the probability of beam-induced electronic excitations using quantum electrodynamics (QED), the most fundamental theory of electromagnetism. We then provide a formalism to compute the degree to which these excitations can increase a material's sputtering rates. Lastly, we show that our new model can accurately predict the sputtering rates in two highly-relevant 2D insulators: hexagonal boron nitride (hBN) and molybdenum disulfide (MoS_2).

This new predictive power can help arm materials engineers with precise atomic-scale control of any 2D material. We also hope that our QED approach can inspire further exploration into the applications of electron beams and the physics of beam-matter interactions.