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Phase transitions in metal-oxide particulate-surface interactions: insights through ab initio study DANIEL FREEDMAN, TOMAS ARIAS, Cornell University — We present results for *ab initio* molecular dynamics calculations of collisions between metal-oxide particulates and metal-oxide surfaces. Detailed examinations of the resulting trajectories suggest particulate internal kinetic energy as a key parameter in obtaining smooth laminar deposition of thin films. Based on *ab initio* calculations and more extensive supporting classical molecular dynamics modelling, we propose a phase-diagram which maps both translational and internal kinetic energy to modes of crystal growth.

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