Multi-Scale Models to Predict the Electrostatic Behavior of Pharmaceutical Powders
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Purpose
Understand the mechanism of tribocharging in particulates (pharmaceutical excipients and API) based on systematic experiments and multi-scale (quantum, bulk) numerical modeling that relates work function (WF) to the tribocharging of granular flow behavior.

Methods
In pharmaceutical formulation processes, particle charging is often a nuisance and can cause problems in the manufacture of products, such as affecting powder flow, and reducing fill. For a fundamental understanding of the powder triboelectrification, it is essential to study charge transfer under well-defined conditions. Hence all experiments were conducted in a humidity controlled glove box at 20% relative humidity. Experiments were conducted with different equipment surfaces viz. PVC, aluminum (Al), Teflon, PMMA with two pharmaceutical excipients and two API’s. The experiments were performed in V-blender at a prescribed speed of 13, 40 and 80rpm. A triboelectric series of pharmaceutical materials was generated. WF was determined using MOPAC, a general-purpose semi-empirical molecular orbital package for the study of solid state and molecular structures and reactions providing band gap and ionization potential of molecules. A discrete element method based model, including charge transfer and screened coulombic forces was developed at particle and bulk scales for particulate flow

Results
Electron transfer has been well established for metal-metal and to some extent for insulator-metal contacts. There is still an ongoing debate for insulator-insulator charging whether the charge carriers are electrons or ions. As per work function hypothesis powders should charge negatively against Al, PMMA surfaces and positively against Teflon surfaces and PVC surfaces. According to the experiments in V-blender both the excipients (lactose, MCC) and API’s charged negatively against PMMA and Aluminum and positively against Teflon and PVC surfaces. In case of blender the charge/mass ratio dropped significantly at speeds greater than 50 rpm.

Conclusion
The sign and magnitude of the charge generated were found in agreement with the difference in work function of the surfaces and primary particles suggesting the charge transfer agents are electrons. The decrease in charge with blender speed was attributed to the poor contact between surface and powder due to centrifuging regime in blender.