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**Dissipation and quantum chemical processes: A case study of anti-wear pad forming zinc polyphophates** MARTIN MUSER, NICHOLAS MOSEY, TOM WOO, University of Western Ontario — It is well established that the typically observed weak dependence of solid friction on sliding velocity must be due to instabilities and molecular hysteresis, as shown in the Prandtl-Tomlinson model. The relevant arguments, however, are by no means limited to plastic or viscoelastic deformations of solids or boundary lubricants, but also apply to chemical hysteresis. Using ab-initio molecular dynamics, we investigate the chemical changes in pure and zinc polyphosphates (ZPs) as a function of their thermomechanical history. ZPs are incorporated in most commercial lubricant mixtures, because they form anti-wear pads on top of rubbing asperities. Under the expected extreme variations of pressure, we find that pure and ZPs undergo changes in atomic coordination number. While the atoms typically move less than 0.1 Angstrom in these processes, large hysteresis effects occur in binding energies and elastic moduli. This implies dissipation due to (hysteresis in) the rearrangment of (local) chemical bonds.

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