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Molecular Mechanisms of Anti-Wear Pad Formation and Function NICHOLAS MOSEY, Department of Chemistry, University of Western Ontario, MARTIN MUESER, Department of Applied Mathematics, University of Western Ontario, TOM WOO, Department of Chemistry, University of Western Ontario — Wear limits the lifespan of many mechanical devices with moving parts. To reduce wear, lubricants are frequently enriched with additives that form protective pads on rubbing surfaces. With first-principles molecular dynamics simulations of pads derived from commercial additives, namely zinc-phosphates, we unravel the molecular origin of how anti-wear pads can form and function. These effects originate from pressure-induced changes in the coordination number of atoms acting as cross-linking agents, in this case zinc, to form chemically connected networks. The proposed mechanism explains a diverse body of experiments and promises to prove useful in the rational design of anti-wear additives that operate on a wider range of surface materials with reduced environmental side-effects.

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