BRIDGING EXPERIMENTS AND COMPUTATIONS TO ADVANCE FRICTION REDUCTION IN LUBRICANT AND COATING SYNERGY

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ABSTRACT

In the realm of material science, the innovative design of materials that effectively minimize friction plays a pivotal role in energy conservation and the reduction of CO_2 emissions. In this study, we explore the synergistic effects of polymeric additive functionalization and silicon doping in diamond-like carbon (DLC) coatings to enhance friction and wear reduction in lubricated systems. We investigate the interaction between nitrogen-containing functional groups in polymeric additives and silicon dopants in DLC coatings. Our research combines experimental observations with computational simulations to unveil the mechanisms behind the observed tribological improvements.

Our findings demonstrate a significant reduction in friction and wear, particularly under severe boundary lubrication conditions. Atomic Force Microscopy (AFM) experiments reveal the formation of a tribofilm, which is absent on standard DLC or with non-functionalized polymers. The tribofilm's presence is pivotal in achieving enhanced lubricity. Additionally, computational studies using density functional theory (DFT) further elucidate the molecular interactions between the copolymers and the Si-DLC surface. The calculations indicate that Si doping enhances the adsorption of functionalized copolymers, promoting chemisorption and the formation of stable bonding, which is pivotal for the development of effective tribofilms.

The study not only shed light on the molecular underpinnings of friction reduction but also pave the way for a high-throughput methodology to identify optimal additive and substrate modifications for desired tribological outcomes. This study thus stands at the forefront of tribological innovation, offering new perspectives on the design of next-generation lubricants and coatings that promise significant advancements in energy efficiency and material longevity.

REFERENCES

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