Contribution ID: **129** Type: **Poster Presentation**

Reactive Molecular Dynamics Simulations of the Atomic Oxygen impact on Poly(2,5)-benzimidazole

In lower Earth orbit (LEO) a spacecraft and its electronics are exposed to an array of different radiation. One of the more destructive types of radiation that takes place in LEO is that of heavy ions. The most abundant heavy ion in the LEO range is atomic oxygen (AO), with a flux rate of $10^{15} AO/cm^2 s$ and energy up to $5eV$. To mitigate or reduce the degree of destruction, various coatings are applied to the devices. Some studies have tested a wide range of coatings from black paint (polyvinyl alcohol) to silicone coatings, among these tests some polymer composites have shown positive results warranting further study. The polymer considered in this work is poly(2,5)-benzimidazole (ABPBI), due to its stability in mechanical and chemical properties at temperatures up to $200^{\circ}C$. To test if ABPBI is a suitable material is a difficult feat given the harsh conditions it would ordinarily experience. The approach taken in this work is to setup a suitable molecular dynamics framework that can be used to compliment experimental setup and then extend studies, beyond the limitations of what can be replicated in the laboratory. The molecular dynamic simulations use ReaxFF, a reactive force field to more accurately evaluate the degradation of ABPBI through hypervelocity AO.

Apply to be considered for a student ; award (Yes / No)?

Yes

Level for award;(Hons, MSc, PhD, N/A)?

MSc

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Session Classification: Poster Session

Track Classification: Track A - Physics of Condensed Matter and Materials