Contribution ID : **255**                                         Type : **Poster Presentation**

# Multiscale Computational Study of Metal (Per)Oxides in Thermoplastic Vulcanizate

Unai Calvo, Fernando Ruipérez, Aizeti Burgoa, Jon Mattin Matxain POLYMAT, Centro Joxe Mari Korte, Avda. Tolosa, 72, 20018, Donostia-San Sebastian, Spain unai.calvo@polymat.eu In this work, we investigate the interactions at the interfaces of metal (per)oxides with thermoplastic vulcanizates (TPVs), specifically focusing on the XHNBR/PA6 system. XHNBR (carboxylated hydrogenated nitrile butadiene rubbre) combined with PA6 (polyamide 6) forms a high-performance TPV with enhanced mechanical and chemical resistance, widely used in automotive and industrial applications. The incorporation of metal (per)oxide nanoparticles plays a key role in crosslinking and improving thermal stability [1-2], yet zinc oxide (ZnO), the most common additive, raises environmental and health concerns. Our study aims to identify a safer alternative by analysing the interactions between metal oxides and both XHNBR and PA6 using quantum chemical calculations, considering cluster and surface model for the metal oxides and different representations of the polymeric materials, including isolated functional groups, monomers, and dimers. The results show that both cluster and surface models exhibit similar interaction patterns with XHNBR and PA6, with predominantly electrostatic interactions, although ZnO presents a slightly more covalent character. To explore the PA6/XHNBR interface, we employ a clustering approach to efficiently sample representative configurations, ensuring a thorough analysis of interfacial interactions. Furthermore, we extend our study to molecular dynamics (MD) simulations of the composite material to predict its mechanical properties [3]. For the development of the methodology for the analyse, we studied the polypropilene (PP) polymeric matrix's mechanical properties. This multiscale approach provides a comprehensive understanding of the role of metal (per)oxides in TPVs, aiding in the design of safer and more efficient formulations. [1] Beitia, A. B. Design and development of high-performance thermoplastic vulcanizates with vibration damping properties, 2020, p 1. [2] Aizeti Burgoa, Ricardo Hernandez, and Jose Luis Vilas. New ways to improv the daping properties in high-performance thermolastic vulcanizates. Polymer International, 69(5):467-475, February 2020. [3] Pervaje, A. K., Psquinelli, M. A., Khan, S. A., & Santiso, E. E. (2022) Multiscale Constitutive Modeling of the Mechanical Properties of Polyropylene Fibers from Molecular Simulation Data. Macromolecules, 55(3), 728-744. https://doi.org/10.1021/acs.macromol.1c00630

**Primary author(s) :** Mr. CALVO, Unai (POLYMAT, Centro Joxe Mari Korte, Avda. Tolosa, 72, 20018, Donostia-San Sebastian, Spain)

**Presenter(s) :** Mr. CALVO, Unai (POLYMAT, Centro Joxe Mari Korte, Avda. Tolosa, 72, 20018, Donostia-San Sebastian, Spain)