INTRODUCTION
Hybrid fibre polymer composites with the integration of nanomaterial constituents (alumina nanoparticles, carbon nanotubes (CNT) in the present work) are enabling the development of new composite material systems with improved thermo-physical and mechanical properties as well as multi-functional material systems. The behaviour and performance of these hybrid fibre composites depend on their processing, and functionalization of the nanomaterials. Nano and low length scale modelling provides an insight to the molecular level interactions of the constituent materials. This paper discusses molecular dynamics modelling of material interactions in hybrid fibre composites. In particular, molecular interactions in a hybrid epoxy fibre composite with epoxy resin, glass fibre and alumina nanoparticles are highlighted.

MOLECULAR MODELING IN HYBRID EPOXY FIBRE COMPOSITES
Hybrid epoxy fibre composites with alumina nanoparticles are formed with nanomaterial integration via either fibre or resin modification [1]. To improve the compatibility of inorganic alumina with epoxy polymer, alumina was functionalized using silane (Tris-2-methoxyethoxy-vinyl-silane). In our prior experimental studies on the mode-I fracture behaviour of these hybrid epoxy composites, the mode-I fracture toughness values were found to be significantly higher with functionalized alumina [2]. The macro level material behaviour depends on the material interactions at the fundamental molecular level. The functionalization of alumina with silane changes the material interface configuration to silane-alumina from the original epon-alumina altering the molecular interfacial energy across the material configurations. Molecular models for the interaction energy of different material interfaces in the hybrid epoxy fibre composite are studied and correlated.

Models of the primary and secondary molecular structures involved are: 1. Epoxy resin based on epoxy end chain with bisphenol-A inner organic group, 2. Curing agent butan-diamine, an amorphous organic compound, 3. Alumina (Aluminium Oxide, Al₂O₃), an inorganic compound, 4) Tris-2-methoxyethoxy-vinyl-silane, an organo-functional group linked to vinyl silane. Interaction energies between two molecular material constituents are studied using molecular layer cells in a vacuum slab. Molecular dynamics simulations were performed using Accelrys [3], a general purpose molecular dynamics modelling analysis software with the COMPASS [3] force field description of the molecular models. Four different molecular layer configurations are investigated as shown in Fig. 1. They are: 1) EPON-Silane, 2) Silane-Alumina, 3) EPON-Alumina, and 4) EPON-EPON. Three primary configurations of EPON (rhomboid, triangle and quasi-quad) composed of 1, 5 and 10 molecules were employed with equivalent lattice structures of organo-silane (T2MEVS) and alumina. The total potential
energies for these molecular systems are obtained after canonical molecular dynamics of the corresponding periodic layer cells.

![Molecular Models of material layers (L-R: EPON-Silane, Silane-Alumina, EPON-Silane, EPON-EPON)](image)

The surface energy at the interface of a layered molecular cell is determined by Eq. 1.

$$E_{A-B} = E_T - (E_A + E_B)$$  \hspace{1cm} (1)

Subscripts A and B denote the two material molecular models in a layered cell, $E_T$ is the total energy, $E_A$ and $E_B$ are the energies of the individual material molecular models; $E_{A-B}$ defines the energy at the interface. The interface interaction energy between EPON-Alumina and EPON-Silane is presented in Fig. 2 for 10 molecular epoxy units. The energy contribution of alumina is negative due to the consistent neglecting of the ionic bond interaction in the molecular models. This net repulsion from the respective models is a measure of the energy between the alumina and either EPON™ or silane (T2MEVS). Silane is observed to have improved adhesion to alumina with a higher interface energy value than EPON-Alumina. This improved adhesion of silane-alumina can be attributed to the increase in the mode-I fracture toughness values due to functionalization observed in our experimental studies [2]. Complete details of the molecular modelling for the interaction energy and property predictions in other hybrid epoxy composites (epoxy-CNT) and comparisons to experimental data are presented in the full paper.

![Interface energy comparison between EPON-Alumina and EPON-Silane](image)

**REFERENCES**


3. Accelrys material studio online manual website: [www.accelrys.com](http://www.accelrys.com)