Contribution ID: **227** Type: **Oral Presentation**

Ab-initio study of ethylene carbonate adsorption on the major α-Al2O3 (0001) surface

Monday, 26 July 2021 15:45 (15 minutes)

Aluminium oxide (α-Al₂O₃) emerged as a potential surface coating material for Li-ion batteries because it has proved to improve the electrochemical performance and capacity upon cycling. It was also considered due to its high thermal conductivity, resistance against extreme temperatures and excellent electric insulation. Despite the intense studies on the surface coating with α-Al₂O₃, there remains a lack of deep understanding of its reactivity towards the electrolyte content. Herein, we report the adsorption of organic solvent, ethylene carbonate (EC) on the major α-Al₂O₃ (0001) surface using density functional theory calculations. During the single EC adsorption, it was found that the molecule prefers to binds with the surface when placed parallel interacting through the carbonyl oxygen. The adsorption energy per EC molecule (*E*_{ads}/EC) was found to increases for parallel interactions and decrease for perpendicular. Upon increasing the surface coverage, we have noted a decrease in surface free energy, thus a decrease in surface stability. Furthermore, it has been observed a decrease in electronic charge transfer as we increase the EC coverage.

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

Yes

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

PhD

Primary author: RAMOGAYANA, Brian (UL)

Co-authors: Dr SANTOS-CARBALLAL, David (Leeds University); MAENETJA, khomotso (University Of Limpopo); Prof. DE LEEUW, Nora. H (Leeds University); NGOEPE, Phuti (University of Limpopo)

Presenter: RAMOGAYANA, Brian (UL)

Session Classification: Physics of Condensed Matter and Materials

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