## Centre for High Performance Computing 2020 National Conference



Contribution ID: 39 Type: Talk

# Interfacial and Morphological phase transitions in Polymeric Materials

Tuesday, 1 December 2020 12:45 (30 minutes)

Confining polymers in thin films causes significant deviations of their structural and dynamical properties from their bulk phase behaviour. In our presentation, we show the different effect of the substrate on binary polymer blends with linear and cyclic architecture, as well as miktoarm star polymers in the presence of explicit solvent, by means of extensive molecular dynamics simulations. In the first case, we discuss the role of enthalpic and entropic factors of the interfacial free energy of the system in determining which species in the blend preferentially adsorbs at the substrate [1,2]. In the case of miktoarm polymers, we vary the solvent-block interaction to monitor the effect on the morphology and self-assembly of the polymer film [3].

[1] G. Pellicane, M. M. Tchoukouegno, G. T. Mola, M. Tsige "Surface enrichment driven by polymer topology" Physical Review E Rapid Communications, 93, 050501 (2016).

[2] F. M. Gaitho and G. Pellicane

"Adsorption of binary polymer mixtures with different topology on a wall" Results in Physics, 12, 975 (2019).

[3] Z. Workineh, G. Pellicane, M. Tsige

"Tuning solvent quality induces morphological phase transitions in miktoarm star polymer films" Macromolecules, 53, 15, 6151 (2020).

#### Student?

No

## Supervisor name

### Supervisor email

Primary author: Prof. PELLICANE, Giuseppe (University of Messina (Italy) and UKZN (South Africa))

Co-authors: Prof. WORKINEH, Zerihun (Bahir Dar University (Ethiopia)); Prof. TSIGE, Mesfin (University of

Akron (US))

Presenter: Prof. PELLICANE, Giuseppe (University of Messina (Italy) and UKZN (South Africa))

Session Classification: HPC Applications

Track Classification: Materials Science