## Modeling strategies for predicting the behavior of nanocomposites: molecular

# dynamics, micromechanics, and finite element approaches

## \*H.K. Lee<sup>1</sup> and B.J. Yang<sup>1</sup>

<sup>1</sup>Department of Civil and Environmental Engineering, Korea Advanced Institute of Science and Technology (KAIST), 291 Daehak-ro, Yuseong-gu, Daejeon 305-701, Republic of Korea

\*Corresponding author: leeh@kaist.ac.kr

Composite materials reinforced by nanoscale inclusions possess unique properties that are often superior over conventional composites (Li et al., 2011). Nanocomposites are thus applicable in numerous industrial fields where lighter weight and higher stiffness are demanding (Barai and Weng, 2011). Whereas the enhanced features are primarily derived from nanoscale fillers, different mechanical and chemical characteristics of the nanocomposites can arise, which restrict precise predictions of the overall behavior of nanocomposites (Yang et al., 2013). With the important issues, an overview on the multiscale framework for predicting the behavior of nanocomposites is presented in this paper in order to provide the ongoing efforts in the relevant fields. Various modeling strategies for nanomaterials are discussed on the basis of different simulation techniques such as molecular dynamics (MD) simulation, micromechanics, and finite element method (MacManus-Driscoll et al., 2008; Park et al., 2010; Barai and Weng, 2011).

**Keywords:** Multiscale framework, Nanocomposites, Molecular dynamics, Micromechanics, Finite element modeling

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