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Computational Material Modeling for Mechanical Properties Prediction of Nanoscale Carbon Based Cementitious Materials

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Abstract : At larger scales, the performance of cementitious materials is impacted by processes occurring at the nanometer scale. These materials boast intricate hierarchical structures with random features that span from the nanometer to millimeter scale. It is fascinating to observe how the nanoscale processes influence the overall behavior and characteristics of these materials. By delving into and manipulating these processes, scientists and engineers can unlock the potential to create more durable and sustainable infrastructure and construction materials. It's like unraveling a hidden tapestry of secrets that hold the key to building stronger and more resilient structures. The present work employs simulations as the computational modeling methodology to predict mechanical properties for carbon/silica based cementitious materials at the molecular/nano scale level. Studies focused on understanding the effect of higher mechanical properties of cementitious materials with carbon silica nanoparticles via Material Studio materials modeling.

Keywords : nanomaterials, SiO_2, carbon black, mechanical properties
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