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Molecular dynamics simulations of Ti and Y impurities in tin-dioxide (SnO2)

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Abstract content
   (Max 300 words)

The present study use classical molecular dynamics technique to report the effect of Ti and Y impurities in tin-dioxide.Empirical Buckingham potential has been chosen to describe the interatomic interations in tin-dioxide. Total energy NPT nose-hoover ensemble at various temperatures has been calculated in order to determine the effect of Ti and Y substitutional defects in tin-dioxide. The results obtained suggest that Ti defect lowers the energy of the host tin-dioxide. The radial distribution functions of Ti doped tin-dioxide suggest the transfromation of anatase to rutile phase at ambiemt temperatures.

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Main supervisor (name and email)
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No

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