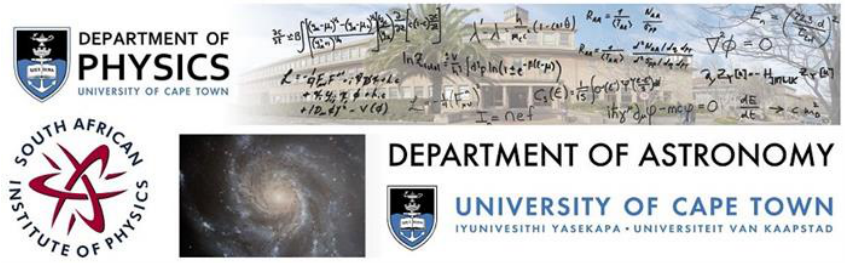

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Structural and dynamical properties of oxygen and cerium vacancies in cerium dioxide

Wednesday, 6 July 2016 16:10 (1h 50m)

Abstract content
   (Max 300 words)
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Structural and dynamical properties of oxygen and cerium vacancies in cerium dioxide are studied using classical molecular dynamics. The formulation uses the Buckingham potential under the NVT ensemble to study these properties. Structural properties are studied using the radial distribution and structure factor functions. The dynamical properties are studied using the time-dependent mean square displacement. Transport properties of both oxygen and cerium vacancies in cerium dioxide are discussed.

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