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Ab initio simulation of effects of structural singularities in aerogel absorption potential

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Abstract

In the present work simulation of Van der Waals potential between helium atom and part of silica aerogel strand by means of ab initio methods was performed. Cell with alpha quartz structure was used as building block of aerogel strand, because it is the most stable structure at low temperature, and only the surface layer of aerogel has been considered. For modeling absorption potential field in plane, summation of potential from individual building blocks has been provided. Two dimensional Van der Waals energy field was calculated for different geometries of aerogel strands. A rather deep potential well has been found in the corner formed due to aerogel strand crossing.

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