

Programme & The Book of Abstracts

Twentieth Annual Conference

YUCOMAT 2018

Herceg Novi, Montenegro, September 3–7, 2018

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TWENTIETH ANNUAL CONFERENCE

YUCOMAT 2018

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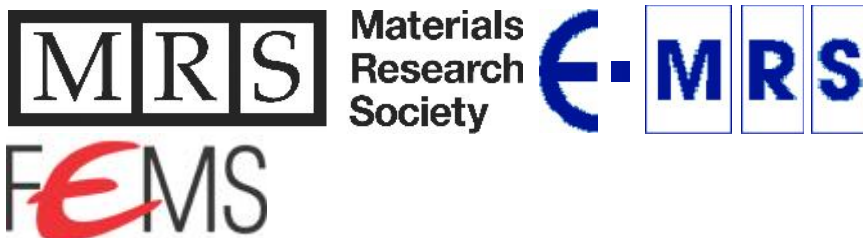
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Prediction of new B₆O structures and their properties using ab initio data mining approach

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Boron suboxide B₆O is the hardest known oxide with high thermal stability, high chemical inertness and high melting temperature which make it applicable for cutting, grinding, drilling and coatings. We used ab initio data mining approach to investigate B₆O system and discover new possible modifications, besides experimentally known R-3m structure (-boron structure). All modifications were optimized by two different ab initio methods using the Crystal17 code. Also, mechanical and electronic properties of experimentally known R-3m structure and new predicted modifications with the B₆O stoichiometry were explored by means of ab initio calculations. Corrections for long-range van der Waals dispersion interactions were taken into account. In this way we could predict the stability of new modifications and possibility to synthesize them using appropriate experimental technique. Obtained results gave us more insight in the B₆O system and open a possibility for ex-panding its use in device applications.

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