Electronic supplementary information (ESI)

Modelling of high-temperature order-disorder phase transitions of non-stoichiometric Mo_2C and Ti_2C from first principles

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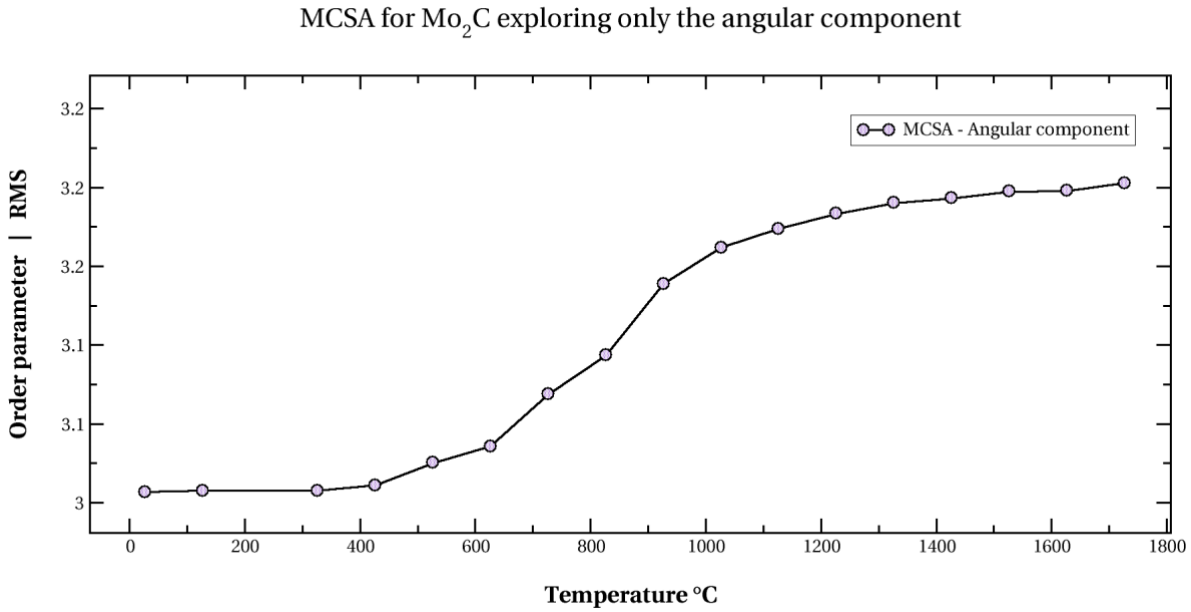

Figure S1. Monte Carlo simulated annealing (MCSA) using only the angular component contribution for Mo_2C.

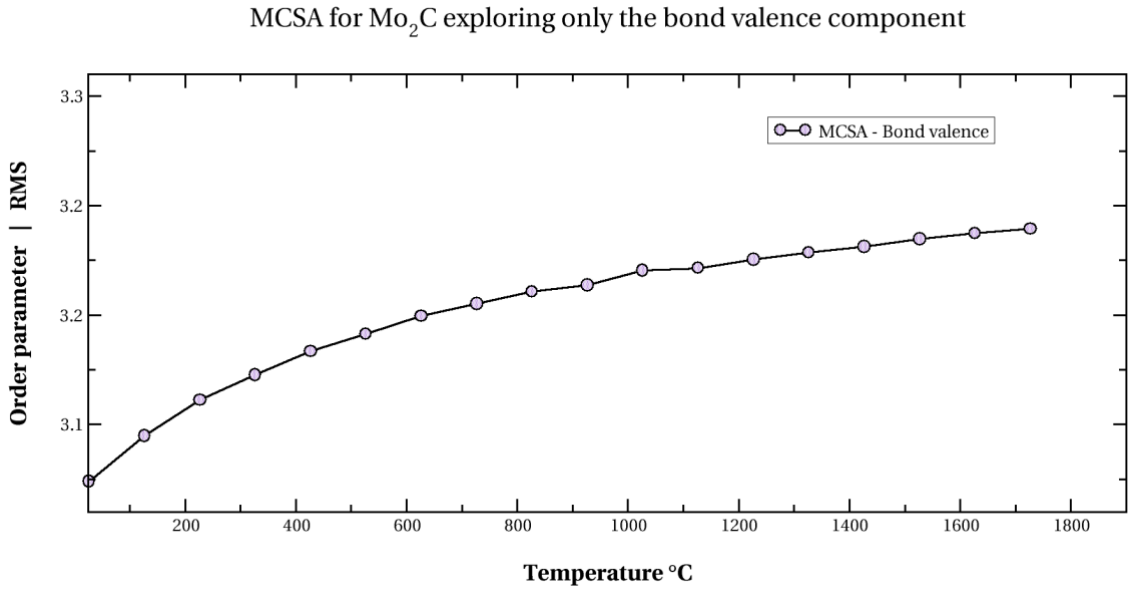

Figure S2. Monte Carlo simulated annealing (MCSA) using only the bond valence component contribution for Mo_2C.

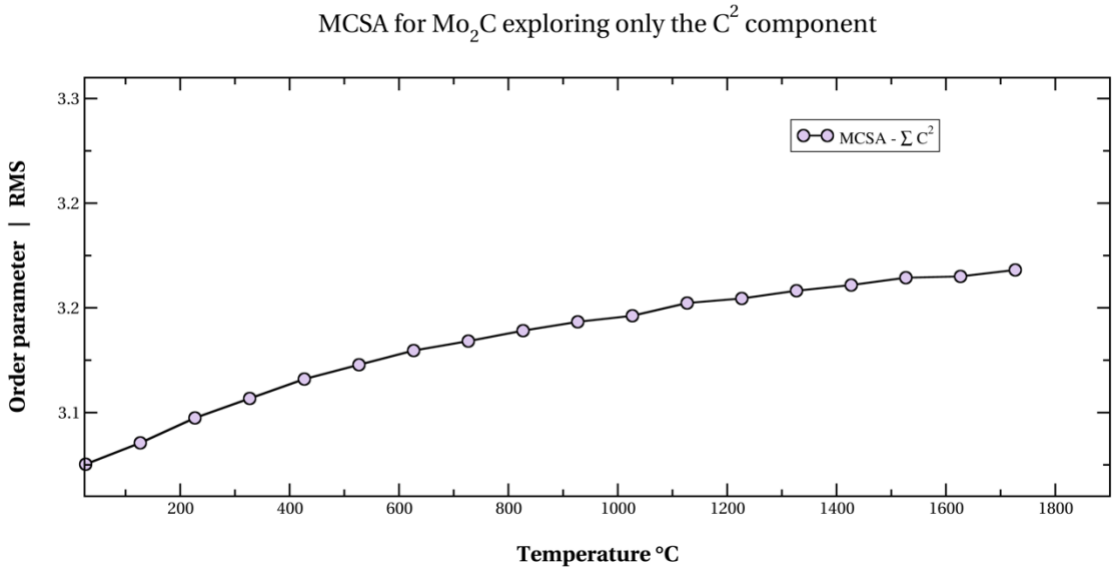

Figure S3. Monte Carlo simulated annealing (MCSA) using only the C^2 summation component contribution for Mo_2C.