

A NOVEL APPROACH TO PARAMETRIC EVALUATION OF THE BUCKINGHAM INTERATOMIC POTENTIAL

Tuesday 24 June 2025 10:00 (30 minutes)

The Modified Buckingham Potential is an empirical phenomenological model that describes interatomic interaction. It offers an alternative to commonly used potentials, such as the Lennard-Jones and Morse potentials. This potential uses a real exponential function to approximate repulsive forces and a negative integer exponential function for attractive forces. In the report, we propose an original method for estimating the parameters of the Buckingham potential. This method is based on representing the potential as a general solution to an equivalent ordinary differential equation, allowing us to estimate a new set of parameters from a linear differential model. The advantage of this approach is that it allows us to find the new unknown parameters by solving a linear algebraic system with constraints, depending on the original parameters.

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Session Classification: Tuesday