Parameter	Content	Data format	Explanation
Objective function	Optimization function	–	Function whose scalar value should be minimized
Initial guess	Material values	array	Initial (scaled) values for the optimization parameters
Additional arguments	Cube parameters	object	Model information from input file
	Load parameters	dictionary	Load parameters from MD-simulations
	Work directory	string	Path to store results
	Evaluation counter	scalar	Counter for the performed function evaltions
method	Nelder mead	–	Mathematical algorithm to perform minimization
bounds	Minimal and maximal material values	array	Limits possible range of optimization parameters
maxiter	Number of maximum iterations	scalar	Limit for optimization iterations