

2023–Kalika-E-B-Verkhovtsev-A-V-Maslov-M-M-et-al–Ni-Cl

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The potential is constructed as a sum of the short-term exponential, long-term r^{-4} power, and the Coulomb potentials:

$$U(r_{ij}) = A_{ij}e^{-\alpha_{ij}r_{ij}} - \frac{C_{ij}}{r_{ij}^4} + \frac{q_i q_j}{4\pi\epsilon_0 r_{ij}}$$

The corresponding parameters of the potential have been determined as described in the above-mentioned manuscript:

	A_{ij} (eV)	α_{ij} (\AA^{-1})	C_{ij} ($\text{eV}\text{\AA}^4$)
Ni-Cl	10715.83	5.034	0.0
Cl-Cl	1439.08	3.494	0.779
Ni-Ni	0.0	0.0	0.0

	q ($ e $)
Ni	1.34
Cl	-0.67

A 7 \AA cutoff was applied for the exponential and power terms of the potential. The Coulomb potential was calculated using the Ewald summation method with the cutoff of 12 \AA .