

# Chemical Simulations

## Chapter 5



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- Details: Qiu, D., et al.<sup>1</sup>

$$G'_{\text{pol},i} = \frac{-166.0}{R_{\text{vdW},i} + \phi + P_1} + \sum^{1,2} \frac{P_2 V_j}{r_{ij}^4} + \sum^{1,3} \frac{P_3 V_j}{r_{ij}^4} + \sum^{1,\geq 4} \frac{P_4 V_j \text{CCF}}{r_{ij}^4}$$

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<sup>1</sup> *J. Phys. Chem. A* **1997**, 101, 3005.