# Dispersion Interaction Energy:



The derivative of Elg :



Define the terms:



Expression of Energy and Force



ReaxFF-lg: Correction of the ReaxFF Reactive Force Field for London Dispersion, with Applications to the Equations of State for Energetic Materials

Lianchi Liu et al. *The Journal of Physical Chemistry* A, **115**, 11016–11022

# Additional Vander-Waal Energy: (For C, H, O, N only)



The derivative of Elg :



Define the terms:



Expression of Energy and Force



Hypervelocity Impact Effect of Molecules from Enceladus' Plume and Titan’s Upper Atmosphere￼on NASA’s Cassini Spectrometer from Reactive Dynamics Simulation

Andres Jaramillo-Botero, et al. *Physical Review Letters* **109**, 213201 (2012)

# New Hydrogen Bond Energy:



The derivative of **EHbond:**



where



Define variables in the code:





Define coefficients for each term:



The final form of EH-bond is: 