

Consequences of Correlation Error

- a. An exact solution of HF equations may still result in a poor description of the molecule, especially D_e .

Molecule	Re (Å)		D (eV)	
	Exp	HF	Exp	HF
H ₂	1.40	1.39	4.75	4.12
N ₂	1.12	1.06	9.9	5.3
O ₂	1.21	1.15	5.08	1.43
F ₂	1.42	1.32	1.68	- 1.37

- b. Note that F₂ is not bound in the HF theory and the correlation error is ~ 24 eV.
- c. Cannot, in general, break a chemical bond in the restricted HF theory. The distance variation of the total energy is most reliable around R_e and least reliable for $R \gg R_e$.