

Front Cover:

C. Cappelli, A. Restrepo et al.

The Role of Spike Protein Mutations in the Infectious Power of SARS-COV-2 Variants: A Molecular Interaction Perspective

classical

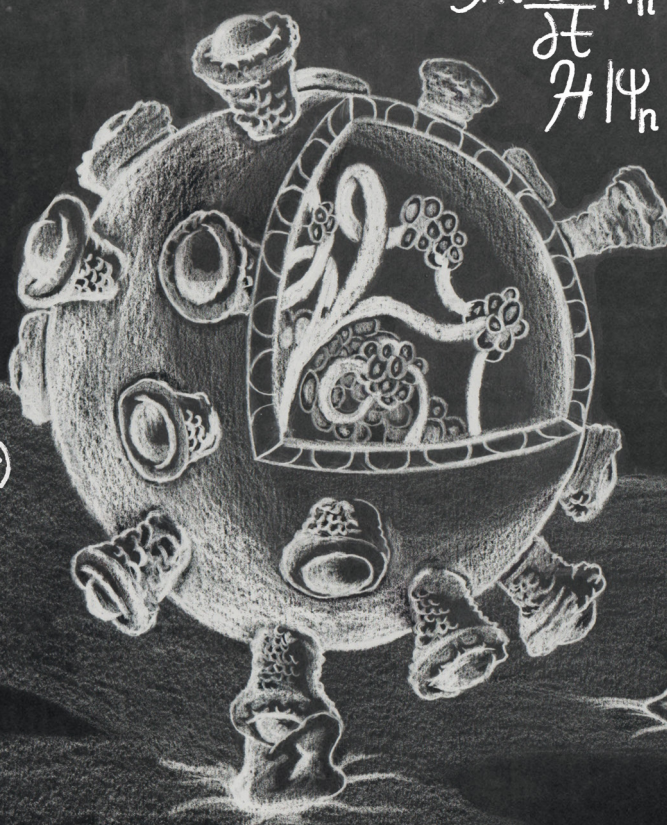
$$V(R) = \sum_{\text{ALL BONDS}} K_b (b - b_0)^2$$

$$+ \sum_{\text{ALL ANGLES}} K_\theta (\theta - \theta_0)^2$$

$$+ \sum_{\text{ALL TORSION ANGLES}} \sum_n K_\phi \cos(n\phi - \phi_0)$$

$$+ \sum_{\text{ALL NONBONDED PAIRS}} \left(\frac{A}{r_{ij}^{12}} - \frac{B}{r_{ij}^6} \right)$$

$$+ \sum_{\text{ALL PARTIAL CHARGES}} \left(\frac{q_i q_j}{\epsilon_0 r_{ij}} \right)$$



Quantum

$$i\hbar \frac{\partial}{\partial t} |\Psi_n(\vec{r}, t)\rangle = \hat{H} |\Psi_n(\vec{r}, t)\rangle$$

$$\hat{H} |\Psi_n(\vec{r}, t)\rangle = E_n |\Psi_n(\vec{r}, t)\rangle$$

$$\frac{f(\vec{r}_c)}{g(\vec{r}_c)}, \frac{H(\vec{r}_c)}{g(\vec{r}_c)}, \frac{|V(\vec{r}_c)|}{g(\vec{r}_c)}$$

$$E_{d \rightarrow a}^{(2)} = -q_d \frac{|\langle \Psi_d | \hat{F} | \Psi_a \rangle|^2}{\epsilon_a - \epsilon_d}$$

$$R_0: \text{WT}=2.5, \Delta=4.7, \beta=4.8, \rho=4.9$$