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Spring 2016

## Construction of multi-state potential energy surfaces for spectroscopy and dynamics

Phalgun Lolur

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$$\hat{H} = \hat{T}_{nuc} + \hat{T}_{el} + \hat{V}_{nuc-nuc} + \hat{V}_{nuc-el} + \hat{V}_{el-el}$$

$$\hat{H} = -\frac{\hbar^2}{2} \sum_{\alpha} \frac{1}{m_{\alpha}} \nabla_{\alpha}^2 - \frac{\hbar^2}{2m_e} \sum_i \nabla_i^2 + \sum_{\alpha} \sum_{\alpha > \beta} \frac{Z_{\alpha} Z_{\beta} e^2}{r_{\alpha\beta}} - \sum_{\alpha} \sum_i \frac{Z_{\alpha} e^2}{r_{i\alpha}} + \sum_{\alpha} \sum_{i > j} \frac{e^2}{r_{ij}}$$

$$\sum_i \nabla_i^2 \equiv \partial^2 / \partial x^2 + \partial^2 / \partial y^2 + \partial^2 / \partial z^2$$

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$$\hat{H}_{el}\Psi_{el}(r;R) = E_{el}\Psi_{el}(r;R)$$

$$\hat{H}_{el} = -\frac{\hbar^2}{2m_e}\sum_i \nabla_i^2 - \sum_\alpha \sum_i \frac{Z_\alpha e^2}{r_{i\alpha}} + \sum_\alpha \sum_{i>j} \frac{e^2}{r_{ij}}$$

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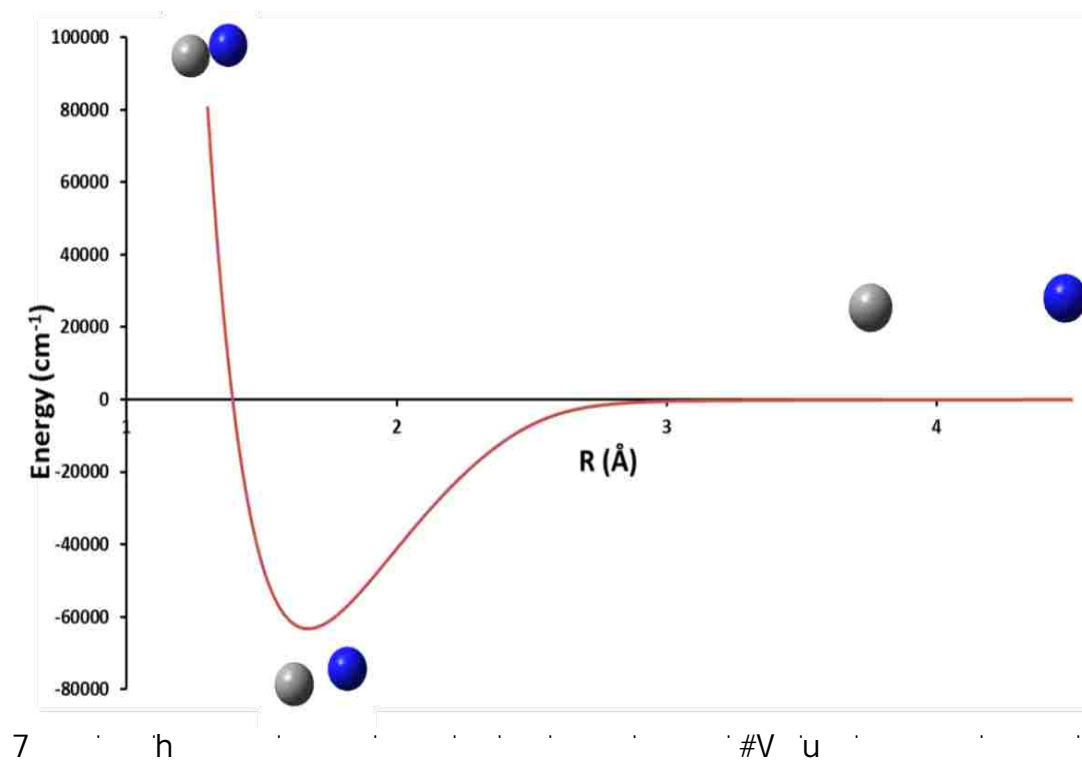
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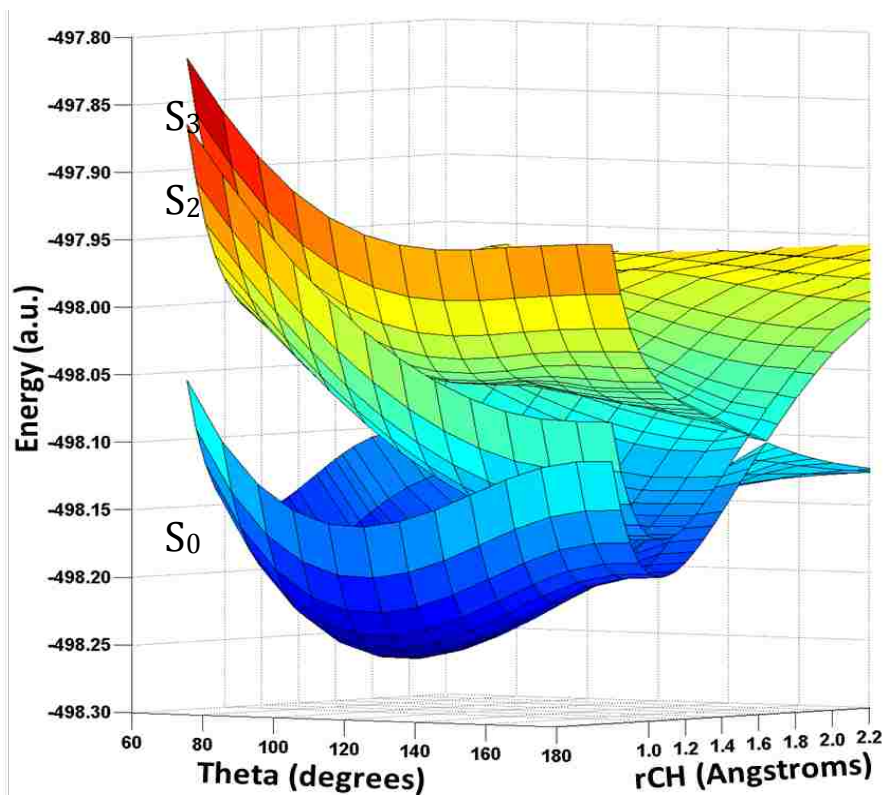
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$$\hat{H}_N \Psi_N(R) = E_R \Psi_N(R)$$

$$\hat{H}_N = -\frac{\hbar^2}{2} \sum_{\alpha} \frac{1}{m_{\alpha}} \nabla_{\alpha}^2 + V(R)$$

$$V(R) = E_{el} + \sum_{\alpha} \sum_{\beta > \alpha} \frac{Z_{\alpha} Z_{\beta} e^2}{r_{\alpha\beta}}$$





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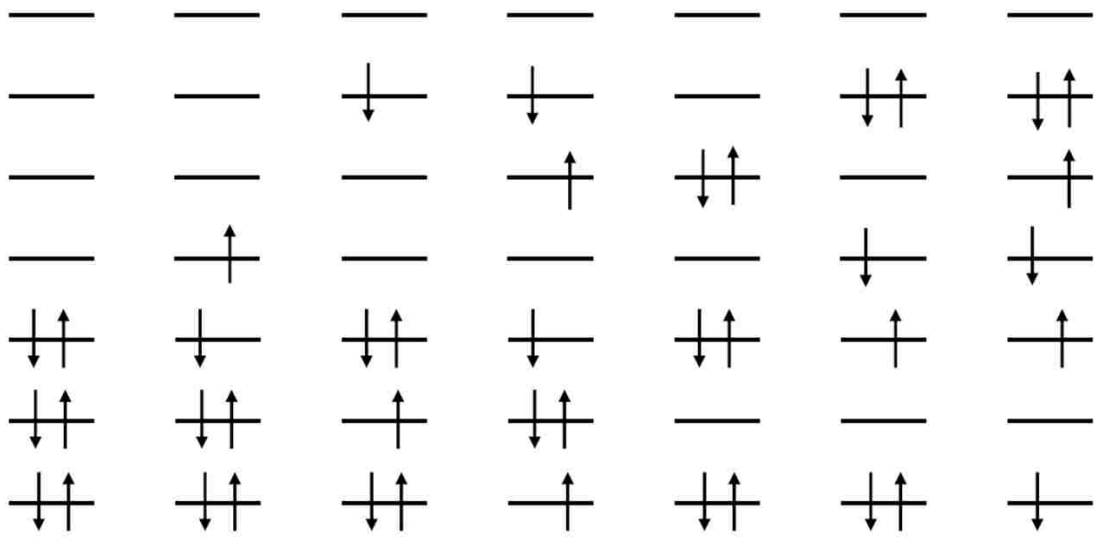
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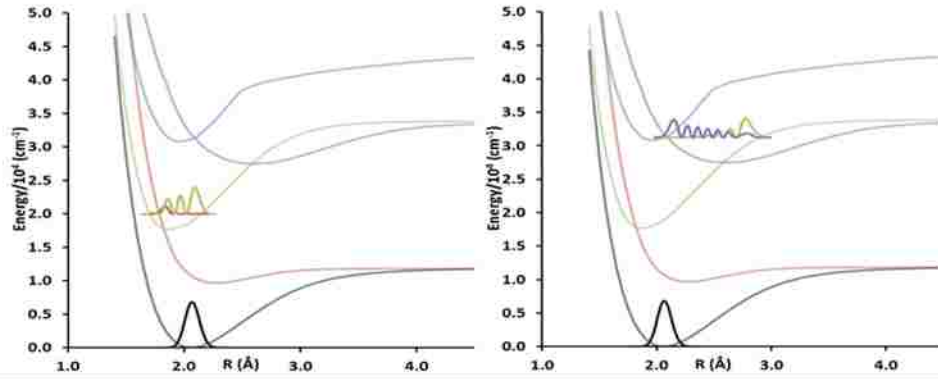
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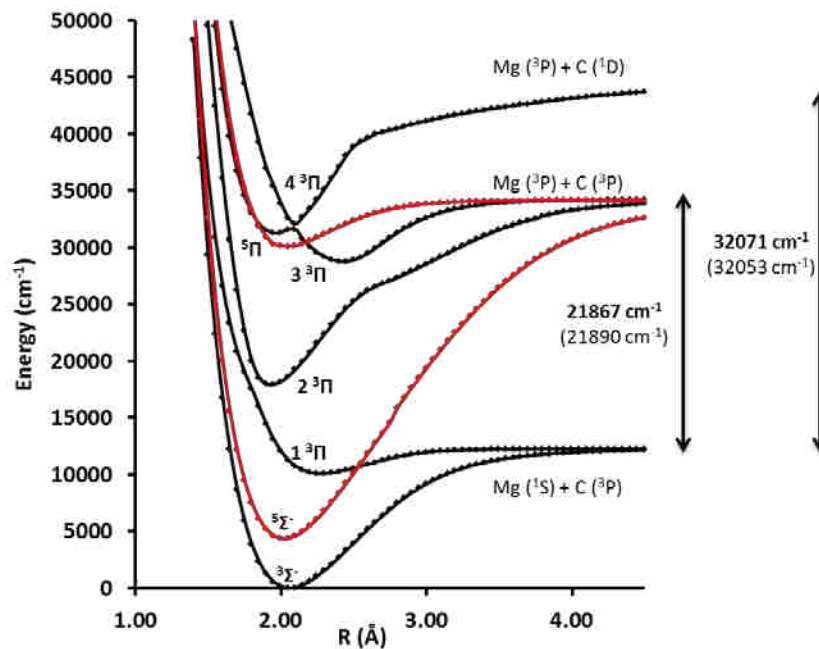
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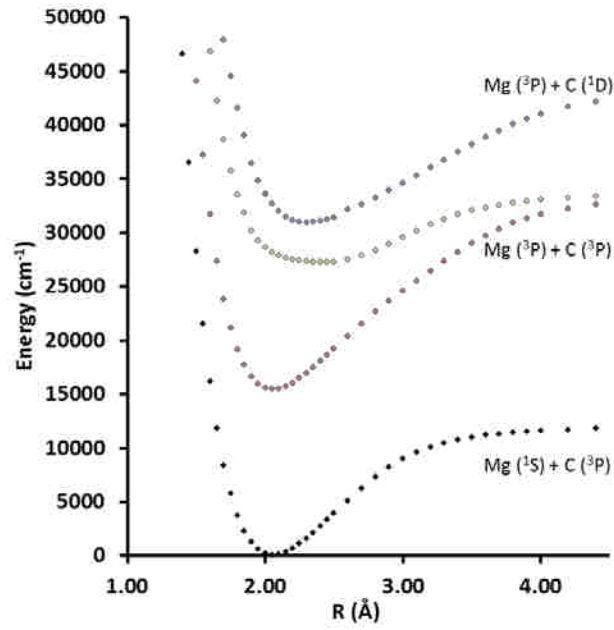
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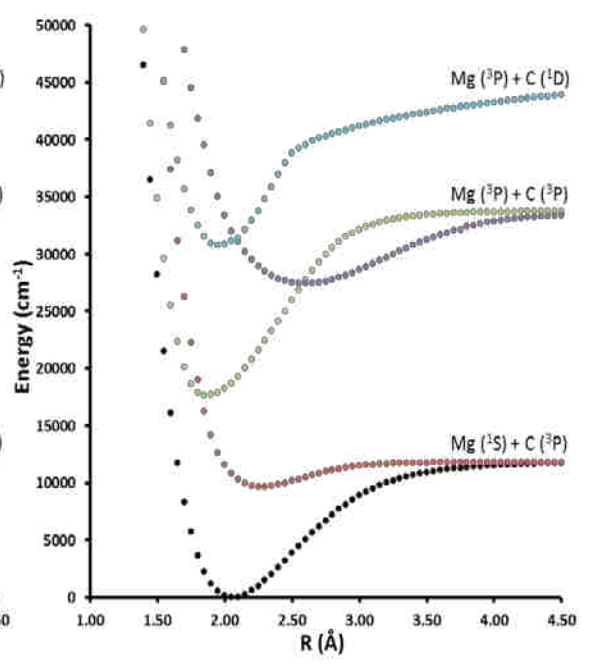
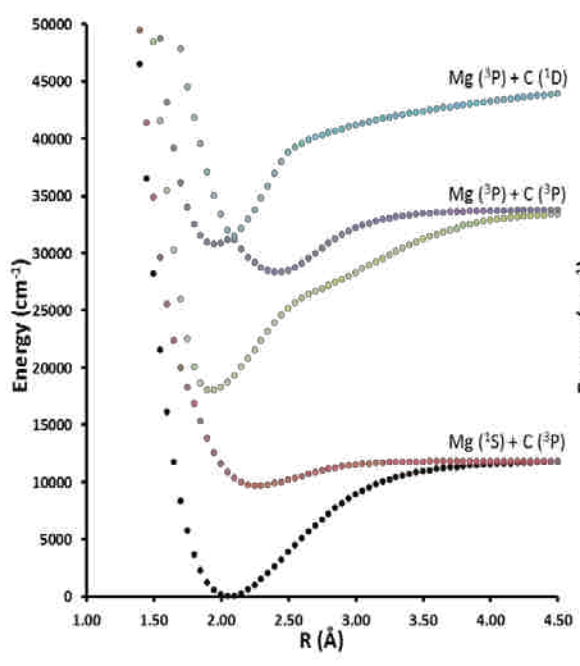


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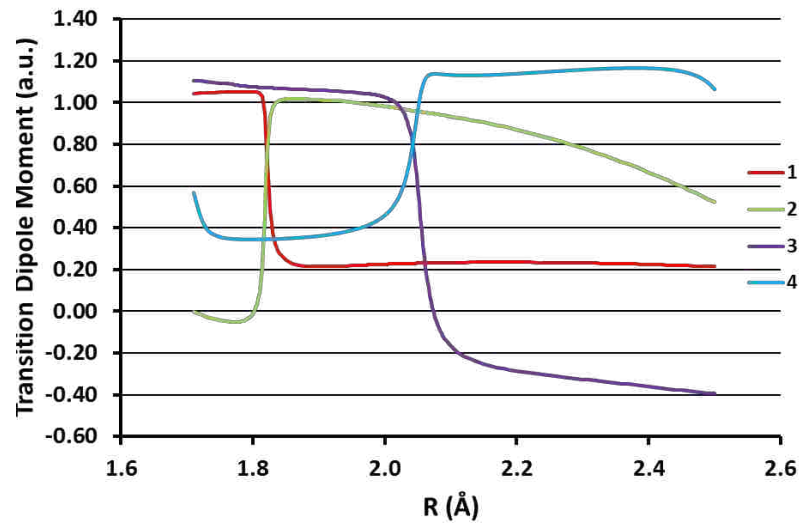
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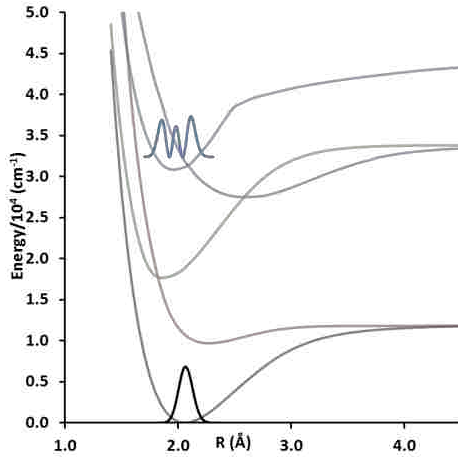
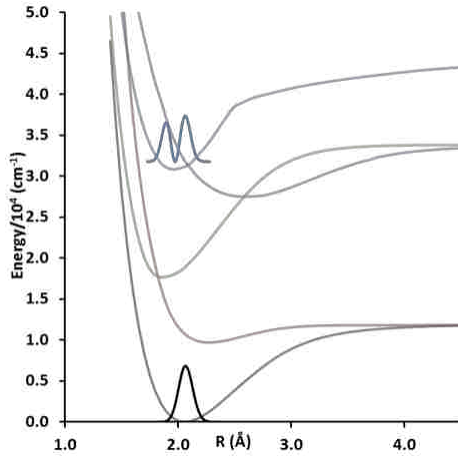
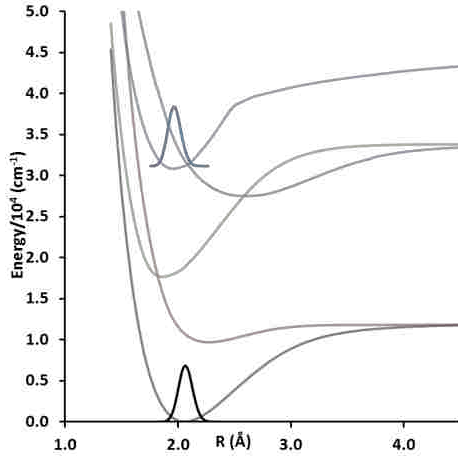
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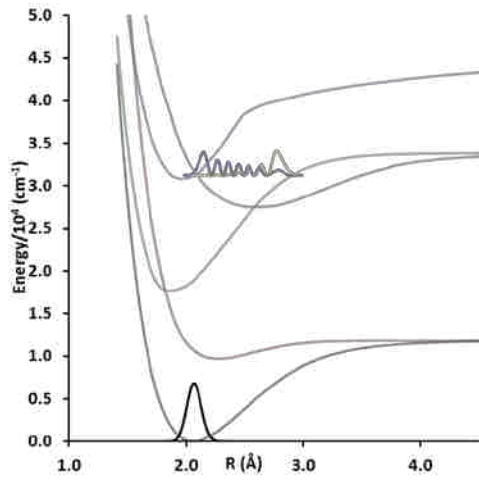
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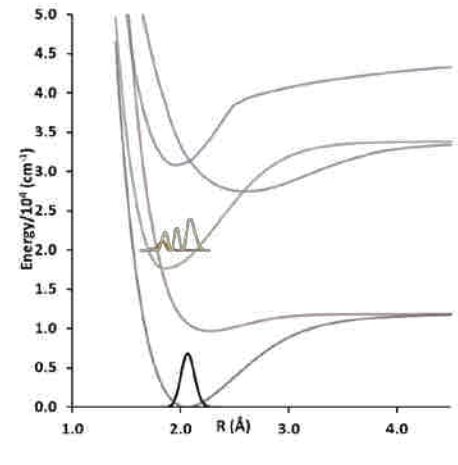
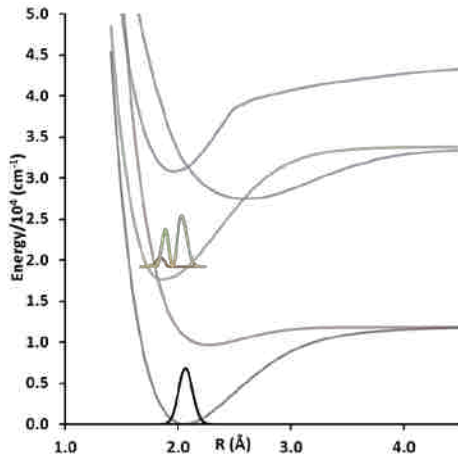
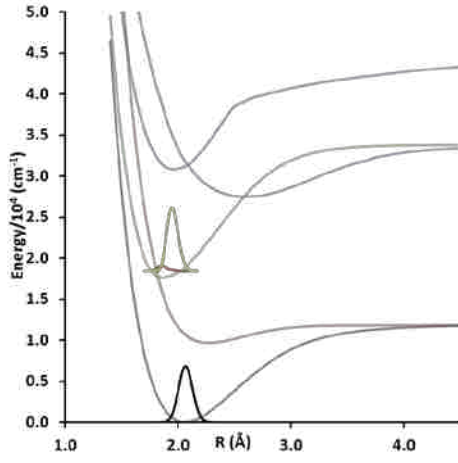
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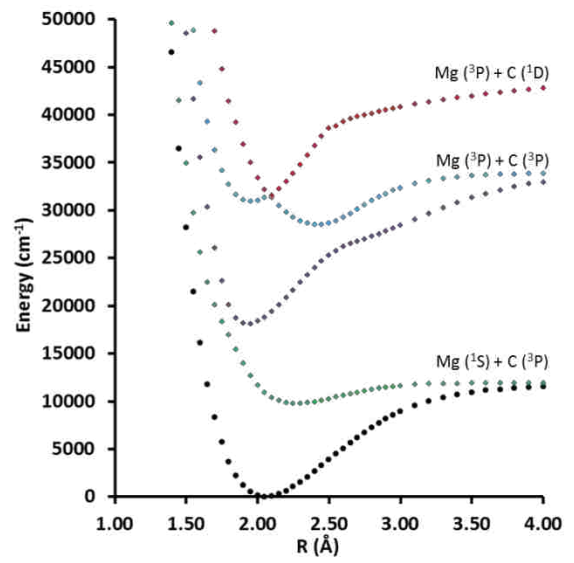
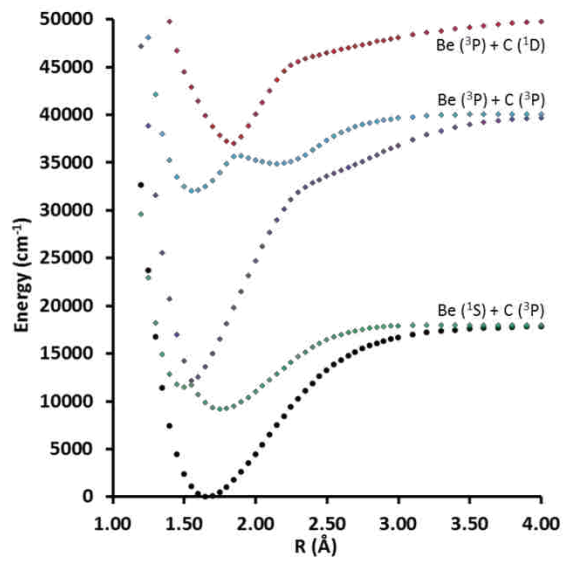
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$$\langle S_0(v_{S_1}, v_{S_2}, v_{S_3}) | \hat{\mathcal{H}}_{SO} | T_1(v_{T_1}, v_{T_2}, v_{T_3}) \rangle = \mathcal{H}_{SO}^{elec} \langle S_0(v_{S_1}, v_{S_2}, v_{S_3}) | T_1(v_{T_1}, v_{T_2}, v_{T_3}) \rangle \quad (1)$$

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$$G(v_1, v_2, v_3) = \omega_1^0 v_1 + \omega_2^0 v_2 + \omega_3^0 v_3 + x_{11}^0 v_1^2 + x_{22}^0 v_2^2 + x_{33}^0 v_3^2 + x_{12}^0 v_1 v_2 + x_{13}^0 v_1 v_3 + x_{23}^0 v_2 v_3 \quad (2)$$

$$\omega_1^0, \omega_2^0, \omega_3^0 \quad \# = \quad = \# \mathbb{C} \quad \# \mathbb{C}$$

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TABLE II. # #=@ #) @

o	U	#	#	#	U	U	7
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TABLE III. Calculated and fit CHBr and CDBr vibrational frequencies in  $\text{cm}^{-1}$ .

$\omega$	U	#	#	#	U	U
		7 <sup>a</sup>	7 <sup>b</sup>	7 <sup>c</sup>	7 <sup>d</sup>	7 <sup>e</sup>
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TABLE IV. # #=# #) #

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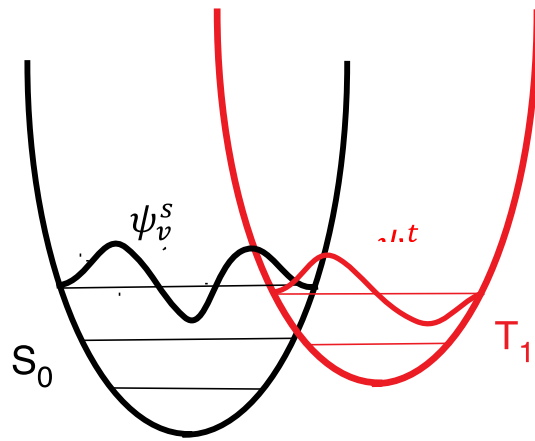
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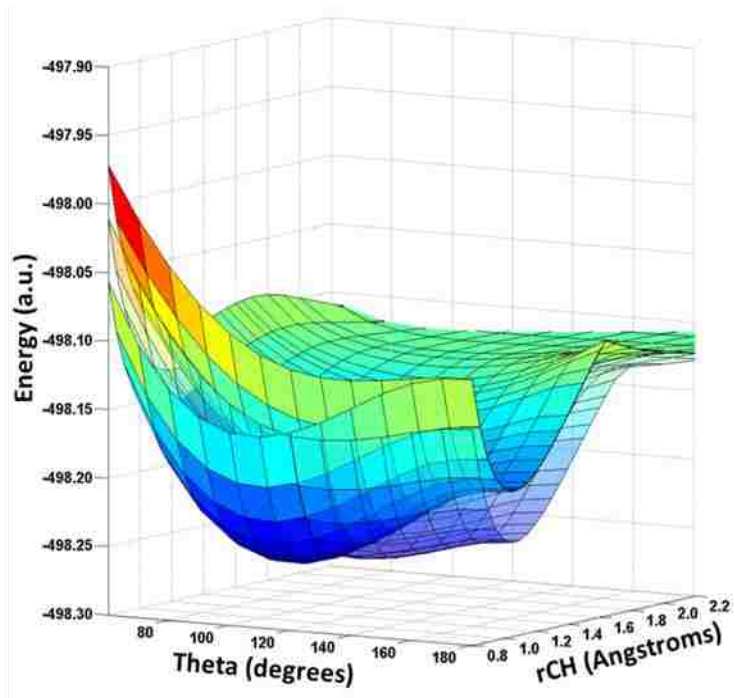
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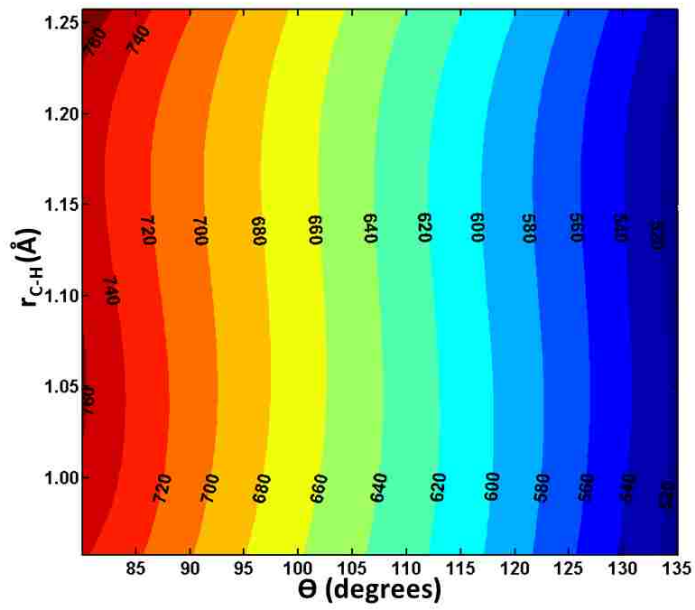
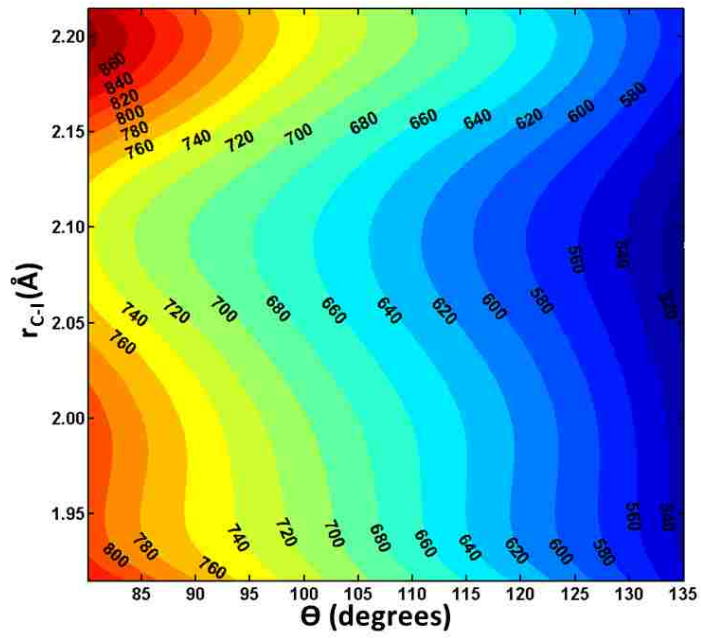
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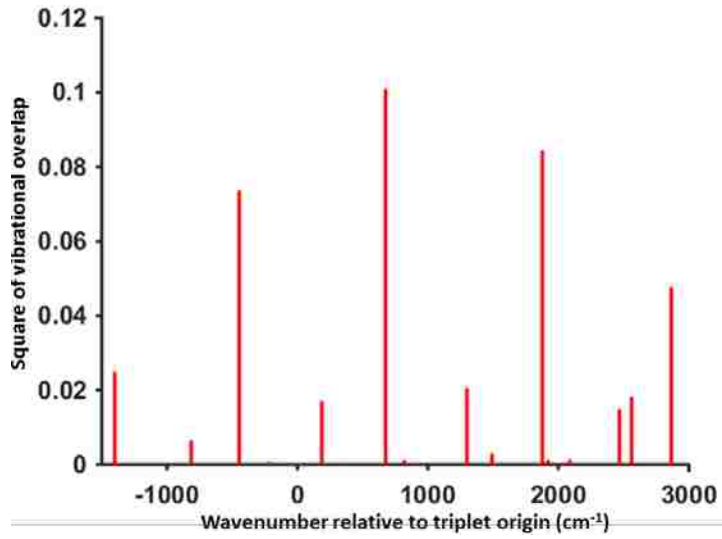
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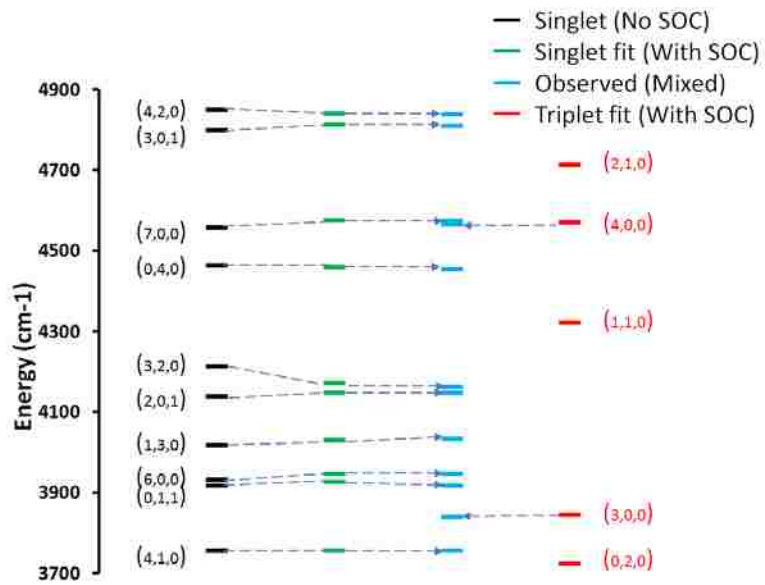
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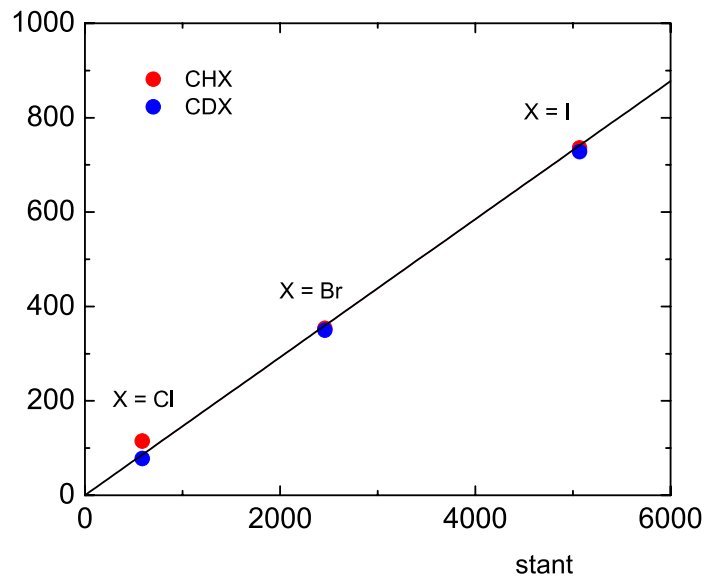
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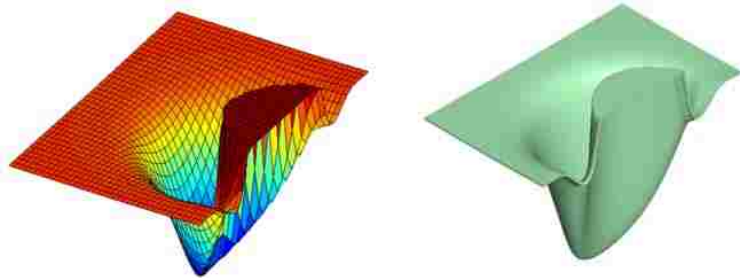
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### III. 3D Printing of Molecular Potential Energy Surface Models

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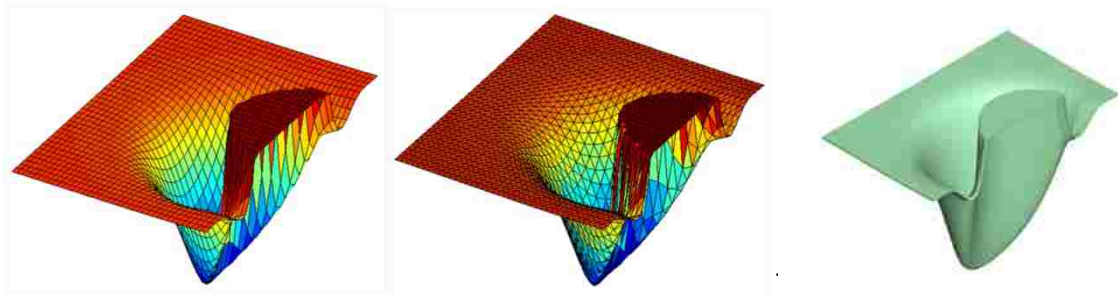
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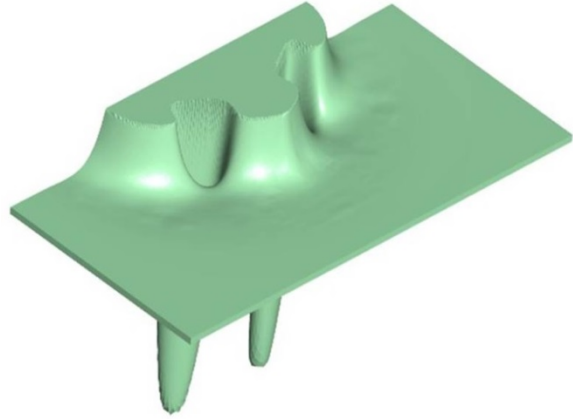
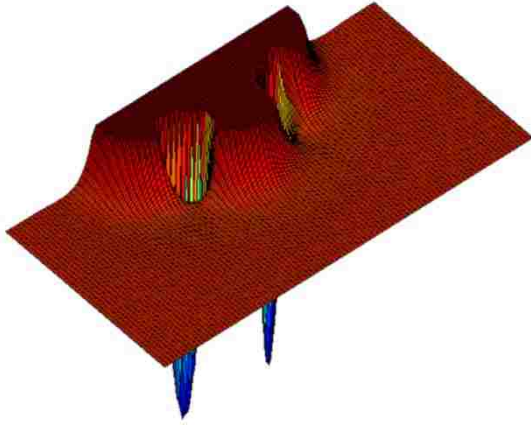
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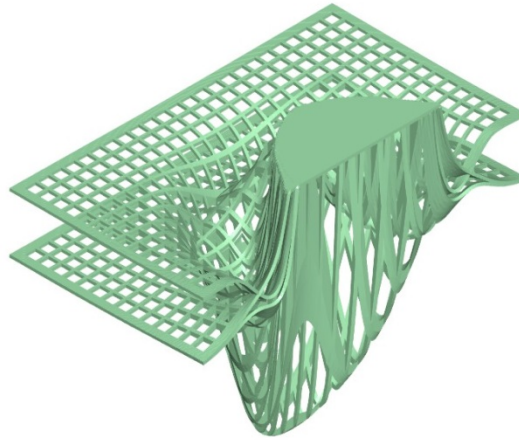
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## VITA

Phalgun Lolur was born on July 9, 1989 in Adoni, India. He obtained his M.S. degree in Chemical Engineering from Missouri University of Science and Technology, Rolla, Missouri in 2013. He has a bachelor's degree in Chemical Engineering from Vellore Institute of Technology (VIT), Vellore, India in 2010. He started his doctoral studies in theoretical chemistry with Dr. Richard Dawes in 2011.

His research was on developing methods for computing accurate multi-state global potential energy surfaces of complex molecular systems, pertaining to combustion, atmospheric and interstellar chemistry. He has six publications in reputed journals like Journal of Chemical Physics, Molecular Physics and Journal of Chemical Education. He also likes to design and develop software for educational purposes occasionally.

Apart from his research, Phalgun has held several executive positions in various student organizations. He attained the honor's list status at Missouri University of Science and Technology in Fall 2014. He has also been actively involved with community service and has volunteered for numerous organizations on multiple occasions.

He received his Ph. D. in Chemistry from Missouri University of Science and Technology in May, 2016.