Inelastic Helium Atom Scattering from the Commensurate Monolayer Solid H$_2$/NaCl(001) L.W. BRUCH, Department of Physics,University of Wisconsin-Madison, F.Y. HANSEN, Department of Chemistry, Technical University of Denmark — A calculation of inelastic low energy helium atomic scattering by a monolayer with one-phonon creation[1] has been adapted to treat the case where the monolayer is the dilated quantum solid H$_2$/NaCl(001). The interactions He-H$_2$ and He-NaCl are rather well known inputs, but the dilated solid presents the most corrugated surface yet treated in such calculations. Progress in performing calculations for the condition of the inelastic scattering experiments[2] will be described. Compared to earlier work, there is remarkable sensitivity to the number of fourier components used to represent the corrugation, the number of coupled channels, and the width of the wave packet.

[1]F. Y. Hansen and L. W. Bruch, J. Chem. Phys. **127**, 204708 (2007)
[2]F. Trager and J. P. Toennies, J. Phys. Chem. B **108**, 14710 (2004)

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