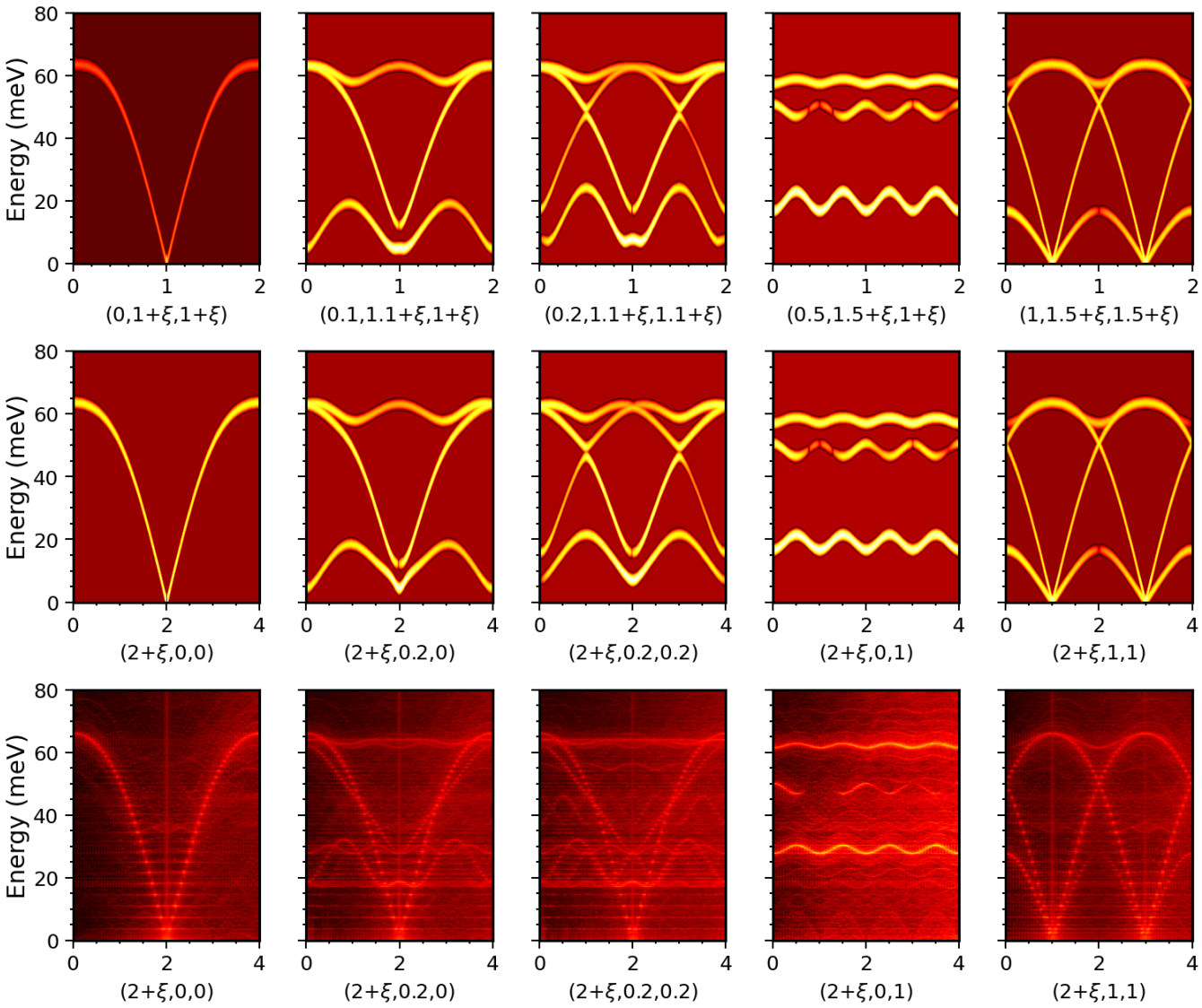

FIG. 7. Comparison of the inelastic neutron scattering dynamical structure factors $S(\mathbf{Q},\omega)$ of silicon computed from DFT and MD. The intensities are plotted in log-scale. top) $S(\mathbf{Q},\omega)$ computed from DFT using the 2-atom primitive cell and a 2x2x2 supercell. middle) $S(\mathbf{Q},\omega)$ computed from DFT using the 8-atom conventional cell and a 1x1x1 supercell. bottom) $S(\mathbf{Q},\omega)$ computed from MD using the 8-atom conventional cell and a 16x2x2 supercell. The top row (2-atom primitive cell) is included to show that the results from the conventional cell are consistent with the primitive cell. The wave vectors where $S(\mathbf{Q},\omega)$ is calculated are under the plots. In the top row, the wave vectors are in the primitive cell basis. In the middle and bottom rows, the wave vectors are given in the conventional cell basis. The discrepencies between the top two rows (DFT calculations) is due to the use of different supercells and underconverged tolerance. Disagreement between the DFT and MD results is likely due to using a classical potential vs. DFT forces as well as all calculations using loose tolerances. The DFT results have been multiplied by the Bose factor and $\frac{1}{\omega}$ to be consistent with the MD results.