

Supplementary Information:

Quo vadis nonlinear optics? An alternative and simple approach to third rank tensors in semiconductors

The complete SBHM bond vector orientation for the perovskite bulk are ($\beta = 90^\circ$):

$$\begin{aligned}
 \hat{b}_1 &= \begin{bmatrix} \frac{1}{2} \sin\left(\frac{19}{18}\beta\right) \\ \frac{\sqrt{3}}{2} \sin\left(\frac{19}{18}\beta\right) \\ \cos\left(\frac{19}{18}\beta\right) \end{bmatrix} & \hat{b}_2 &= \begin{bmatrix} \frac{1}{2} \sin\left(\frac{17}{18}\beta\right) \\ \frac{\sqrt{3}}{2} \sin\left(\frac{17}{18}\beta\right) \\ \cos\left(\frac{17}{18}\beta\right) \end{bmatrix} & \hat{b}_3 &= \begin{bmatrix} -\frac{1}{2} \sin\left(\frac{19}{18}\beta\right) \\ -\frac{\sqrt{3}}{2} \sin\left(\frac{19}{18}\beta\right) \\ \cos\left(\frac{19}{18}\beta\right) \end{bmatrix} \\
 \hat{b}_4 &= \begin{bmatrix} -\frac{1}{2} \sin\left(\frac{17}{18}\beta\right) \\ -\frac{\sqrt{3}}{2} \sin\left(\frac{17}{18}\beta\right) \\ \cos\left(\frac{17}{18}\beta\right) \end{bmatrix} & \hat{b}_5 &= \begin{bmatrix} \frac{\sqrt{3}}{2} \sin\left(\frac{17}{18}\beta\right) \\ \frac{1}{2} \sin\left(\frac{17}{18}\beta\right) \\ \cos\left(\frac{17}{18}\beta\right) \end{bmatrix} & \hat{b}_6 &= \begin{bmatrix} \frac{\sqrt{3}}{2} \sin\left(\frac{19}{18}\beta\right) \\ \frac{1}{2} \sin\left(\frac{19}{18}\beta\right) \\ \cos\left(\frac{19}{18}\beta\right) \end{bmatrix} \\
 \hat{b}_7 &= \begin{bmatrix} -\frac{1}{2} \sin\left(\frac{17}{18}\beta\right) \\ \frac{\sqrt{3}}{2} \sin\left(\frac{17}{18}\beta\right) \\ \cos\left(\frac{17}{18}\beta\right) \end{bmatrix} & \hat{b}_8 &= \begin{bmatrix} -\frac{1}{2} \sin\left(\frac{19}{18}\beta\right) \\ \frac{\sqrt{3}}{2} \sin\left(\frac{19}{18}\beta\right) \\ \cos\left(\frac{19}{18}\beta\right) \end{bmatrix} & \hat{b}_9 &= \begin{bmatrix} -\frac{\sqrt{3}}{2} \sin\left(\frac{19}{18}\beta\right) \\ -\frac{1}{2} \sin\left(\frac{19}{18}\beta\right) \\ \cos\left(\frac{19}{18}\beta\right) \end{bmatrix} \\
 \hat{b}_{10} &= \begin{bmatrix} -\frac{\sqrt{3}}{2} \sin\left(\frac{19}{18}\beta\right) \\ -\frac{1}{2} \sin\left(\frac{19}{18}\beta\right) \\ \cos\left(\frac{19}{18}\beta\right) \end{bmatrix} & \hat{b}_{11} &= \begin{bmatrix} \frac{1}{2} \sin\left(\frac{17}{18}\beta\right) \\ -\frac{\sqrt{3}}{2} \sin\left(\frac{17}{18}\beta\right) \\ \cos\left(\frac{17}{18}\beta\right) \end{bmatrix} & \hat{b}_{12} &= \begin{bmatrix} \frac{1}{2} \sin\left(\frac{19}{18}\beta\right) \\ -\frac{\sqrt{3}}{2} \sin\left(\frac{19}{18}\beta\right) \\ \cos\left(\frac{19}{18}\beta\right) \end{bmatrix} \\
 \hat{b}_{13} &= \begin{bmatrix} -\frac{\sqrt{3}}{2} \sin\left(\frac{17}{18}\beta\right) \\ \frac{1}{2} \sin\left(\frac{17}{18}\beta\right) \\ \cos\left(\frac{17}{18}\beta\right) \end{bmatrix} & \hat{b}_{14} &= \begin{bmatrix} -\frac{\sqrt{3}}{2} \sin\left(\frac{19}{18}\beta\right) \\ \frac{1}{2} \sin\left(\frac{19}{18}\beta\right) \\ \cos\left(\frac{19}{18}\beta\right) \end{bmatrix} & \hat{b}_{15} &= \begin{bmatrix} \frac{\sqrt{3}}{2} \sin\left(\frac{19}{18}\beta\right) \\ -\frac{1}{2} \sin\left(\frac{19}{18}\beta\right) \\ \cos\left(\frac{19}{18}\beta\right) \end{bmatrix} \\
 \hat{b}_{16} &= \begin{bmatrix} \frac{\sqrt{3}}{2} \sin\left(\frac{17}{18}\beta\right) \\ -\frac{1}{2} \sin\left(\frac{17}{18}\beta\right) \\ \cos\left(\frac{17}{18}\beta\right) \end{bmatrix} & \hat{b}_{17} &= \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} & \hat{b}_{18} &= \begin{bmatrix} 0 \\ 0 \\ -1 \end{bmatrix}
 \end{aligned}$$

$$\begin{aligned}
 \hat{b}_{19} &= -\hat{b}_1, \quad \hat{b}_{20} = -\hat{b}_2, \quad \hat{b}_{21} = -\hat{b}_3, \quad \hat{b}_{22} = -\hat{b}_4, \quad \hat{b}_{23} = -\hat{b}_5, \\
 \hat{b}_{24} &= -\hat{b}_6, \quad \hat{b}_{25} = -\hat{b}_7, \quad \hat{b}_{26} = -\hat{b}_8, \quad \hat{b}_{27} = -\hat{b}_9, \quad \hat{b}_{28} = -\hat{b}_{10}, \\
 \hat{b}_{29} &= -\hat{b}_{11}, \quad \hat{b}_{30} = -\hat{b}_{12}, \quad \hat{b}_{31} = -\hat{b}_{13}, \quad \hat{b}_{32} = -\hat{b}_{14}, \quad \hat{b}_{33} = -\hat{b}_{15}, \\
 \hat{b}_{34} &= -\hat{b}_{16}, \quad \hat{b}_{35} = -\hat{b}_{17}, \quad \hat{b}_{36} = -\hat{b}_{18}.
 \end{aligned}$$

The complete SBHM bond vector orientation for the perovskite surface are ($\beta = 90^\circ$):

$$\begin{aligned}
\hat{b}_1 &= \begin{bmatrix} \frac{1}{2} \sin\left(\frac{19}{18}\beta\right) \\ \frac{\sqrt{3}}{2} \sin\left(\frac{19}{18}\beta\right) \\ \cos\left(\frac{19}{18}\beta\right) \end{bmatrix} & \hat{b}_2 &= \begin{bmatrix} \frac{1}{2} \sin\left(\frac{17}{18}\beta\right) \\ \frac{\sqrt{3}}{2} \sin\left(\frac{17}{18}\beta\right) \\ \cos\left(\frac{17}{18}\beta\right) \end{bmatrix} & \hat{b}_3 &= \begin{bmatrix} -\frac{1}{2} \sin\left(\frac{19}{18}\beta\right) \\ -\frac{\sqrt{3}}{2} \sin\left(\frac{19}{18}\beta\right) \\ \cos\left(\frac{19}{18}\beta\right) \end{bmatrix} \\
\hat{b}_4 &= \begin{bmatrix} -\frac{1}{2} \sin\left(\frac{17}{18}\beta\right) \\ -\frac{\sqrt{3}}{2} \sin\left(\frac{17}{18}\beta\right) \\ \cos\left(\frac{17}{18}\beta\right) \end{bmatrix} & \hat{b}_5 &= \begin{bmatrix} \frac{\sqrt{3}}{2} \sin\left(\frac{17}{18}\beta\right) \\ \frac{1}{2} \sin\left(\frac{17}{18}\beta\right) \\ \cos\left(\frac{17}{18}\beta\right) \end{bmatrix} & \hat{b}_6 &= \begin{bmatrix} \frac{\sqrt{3}}{2} \sin\left(\frac{19}{18}\beta\right) \\ \frac{1}{2} \sin\left(\frac{19}{18}\beta\right) \\ \cos\left(\frac{19}{18}\beta\right) \end{bmatrix} \\
\hat{b}_7 &= \begin{bmatrix} -\frac{1}{2} \sin\left(\frac{17}{18}\beta\right) \\ \frac{\sqrt{3}}{2} \sin\left(\frac{17}{18}\beta\right) \\ \cos\left(\frac{17}{18}\beta\right) \end{bmatrix} & \hat{b}_8 &= \begin{bmatrix} -\frac{1}{2} \sin\left(\frac{19}{18}\beta\right) \\ \frac{\sqrt{3}}{2} \sin\left(\frac{19}{18}\beta\right) \\ \cos\left(\frac{19}{18}\beta\right) \end{bmatrix} & \hat{b}_9 &= \begin{bmatrix} -\frac{\sqrt{3}}{2} \sin\left(\frac{19}{18}\beta\right) \\ -\frac{1}{2} \sin\left(\frac{19}{18}\beta\right) \\ \cos\left(\frac{19}{18}\beta\right) \end{bmatrix} \\
\hat{b}_{10} &= \begin{bmatrix} -\frac{\sqrt{3}}{2} \sin\left(\frac{19}{18}\beta\right) \\ -\frac{1}{2} \sin\left(\frac{19}{18}\beta\right) \\ \cos\left(\frac{19}{18}\beta\right) \end{bmatrix} & \hat{b}_{11} &= \begin{bmatrix} \frac{1}{2} \sin\left(\frac{17}{18}\beta\right) \\ -\frac{\sqrt{3}}{2} \sin\left(\frac{17}{18}\beta\right) \\ \cos\left(\frac{17}{18}\beta\right) \end{bmatrix} & \hat{b}_{12} &= \begin{bmatrix} \frac{1}{2} \sin\left(\frac{19}{18}\beta\right) \\ -\frac{\sqrt{3}}{2} \sin\left(\frac{19}{18}\beta\right) \\ \cos\left(\frac{19}{18}\beta\right) \end{bmatrix} \\
\hat{b}_{13} &= \begin{bmatrix} -\frac{\sqrt{3}}{2} \sin\left(\frac{17}{18}\beta\right) \\ \frac{1}{2} \sin\left(\frac{17}{18}\beta\right) \\ \cos\left(\frac{17}{18}\beta\right) \end{bmatrix} & \hat{b}_{14} &= \begin{bmatrix} -\frac{\sqrt{3}}{2} \sin\left(\frac{19}{18}\beta\right) \\ \frac{1}{2} \sin\left(\frac{19}{18}\beta\right) \\ \cos\left(\frac{19}{18}\beta\right) \end{bmatrix} & \hat{b}_{15} &= \begin{bmatrix} \frac{\sqrt{3}}{2} \sin\left(\frac{19}{18}\beta\right) \\ -\frac{1}{2} \sin\left(\frac{19}{18}\beta\right) \\ \cos\left(\frac{19}{18}\beta\right) \end{bmatrix} \\
\hat{b}_{16} &= \begin{bmatrix} \frac{\sqrt{3}}{2} \sin\left(\frac{17}{18}\beta\right) \\ -\frac{1}{2} \sin\left(\frac{17}{18}\beta\right) \\ \cos\left(\frac{17}{18}\beta\right) \end{bmatrix} & \hat{b}_{17} &= \begin{bmatrix} \frac{\sqrt{3}}{2} \sin\left(\frac{35}{18}\beta\right) \\ \frac{1}{2} \sin\left(\frac{35}{18}\beta\right) \\ \cos\left(\frac{35}{18}\beta\right) \end{bmatrix} & \hat{b}_{18} &= \begin{bmatrix} \frac{\sqrt{3}}{2} \sin\left(\frac{35}{18}\beta\right) \\ -\frac{1}{2} \sin\left(\frac{35}{18}\beta\right) \\ \cos\left(\frac{35}{18}\beta\right) \end{bmatrix} \\
\hat{b}_{19} &= \begin{bmatrix} -\frac{\sqrt{3}}{2} \sin\left(\frac{35}{18}\beta\right) \\ -\frac{1}{2} \sin\left(\frac{35}{18}\beta\right) \\ \cos\left(\frac{35}{18}\beta\right) \end{bmatrix} & \hat{b}_{20} &= \begin{bmatrix} -\frac{\sqrt{3}}{2} \sin\left(\frac{35}{18}\beta\right) \\ \frac{1}{2} \sin\left(\frac{35}{18}\beta\right) \\ \cos\left(\frac{35}{18}\beta\right) \end{bmatrix}
\end{aligned}$$

$$\begin{aligned}
\hat{b}_{21} &= -\hat{b}_1, \quad \hat{b}_{22} = -\hat{b}_2, \quad \hat{b}_{23} = -\hat{b}_3, \quad \hat{b}_{24} = -\hat{b}_4, \quad \hat{b}_{25} = -\hat{b}_5, \\
\hat{b}_{26} &= -\hat{b}_6, \quad \hat{b}_{27} = -\hat{b}_7, \quad \hat{b}_{28} = -\hat{b}_8, \quad \hat{b}_{29} = -\hat{b}_9, \quad \hat{b}_{30} = -\hat{b}_{10}, \\
\hat{b}_{31} &= -\hat{b}_{11}, \quad \hat{b}_{32} = -\hat{b}_{12}, \quad \hat{b}_{33} = -\hat{b}_{13}, \quad \hat{b}_{34} = -\hat{b}_{14}, \quad \hat{b}_{35} = -\hat{b}_{15}, \\
\hat{b}_{36} &= -\hat{b}_{16}, \quad \hat{b}_{37} = -\hat{b}_{17}, \quad \hat{b}_{38} = -\hat{b}_{18}, \quad \hat{b}_{39} = -\hat{b}_{19}, \quad \hat{b}_{40} = -\hat{b}_{20}.
\end{aligned}$$