Visualization of Structure-Property Relationships: Spanning the Length Scales (nano to macro)

http://www.jwave.vt.edu/~rkriz/Pubs/NSF_SEVC/NSF_sevc.doc

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by

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Description (100 words)

Recent development of networked collaborative immersive software [1-3] allows more accurate visual analysis of complex connected wave-velocity surfaces propagating through anisotropic crystals. Existing topologies, used for sub-classification within orthorhombic symmetry [4-6], were studied using these immersive tools. From Christoffel's equation the fourth order elastic stiffness tensor, C_{ijkl}, uniquely defines these topologies where the collection of all wave speeds, v, (topology) and their vibration directions, $\square_k$, correspond to the wave propagation direction, $\square_k$, and color is defined by $\square_k \square_k$ [7]. Together both topology and color uniquely represent C_{ijkl} for Ca[HCOO]2. Insight occurs when the observer is "immersed" inside the crystal (nano-structure) and the wave velocity (macro-property) topology. Polar covalent bond orientations are seen to align along stiffer directions where faster longitudinal wave speeds appear as purple bulges.

REFERENCES

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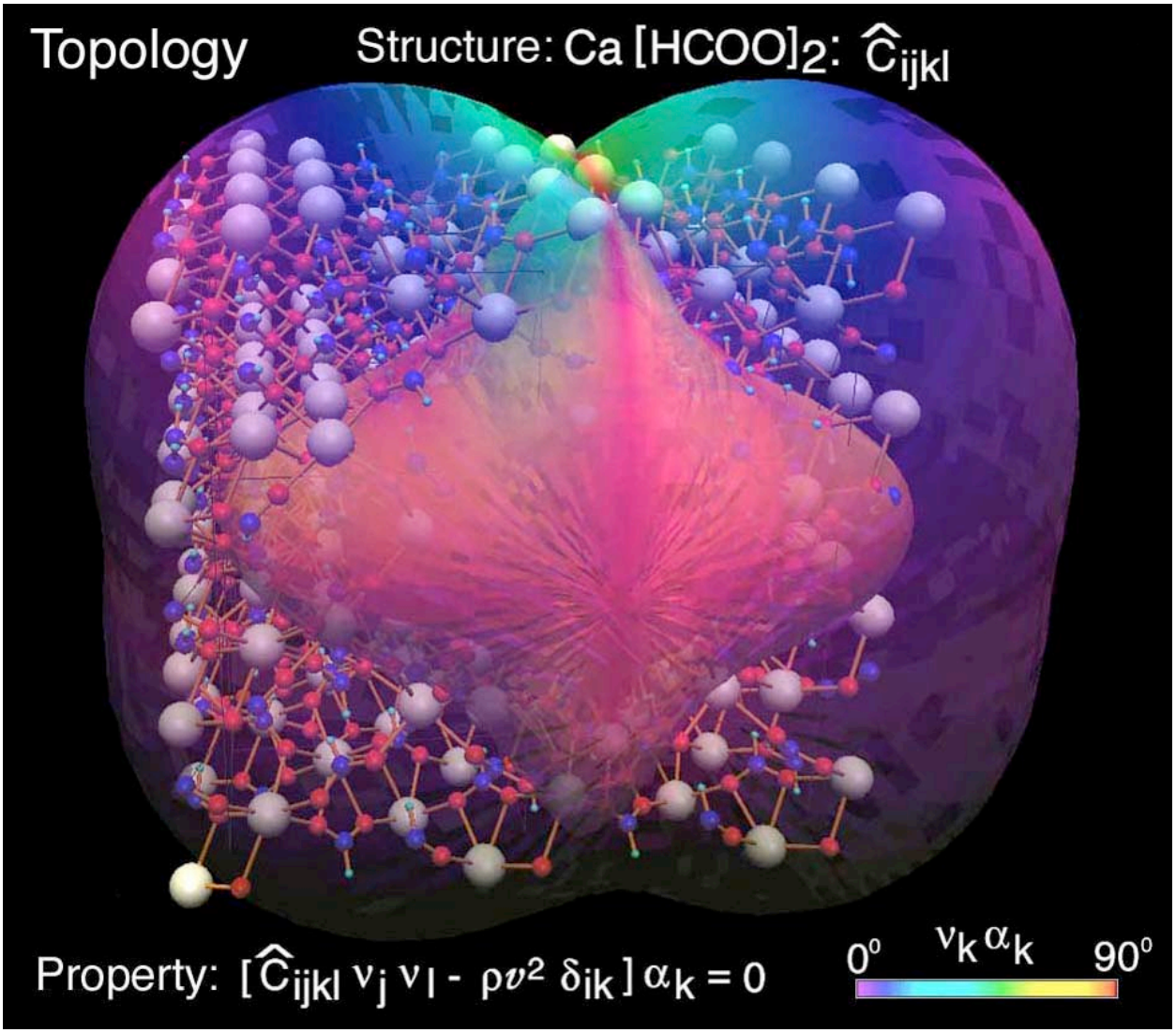

Figure 1a. Nano-Macro Topology for Ca[HCOO]2

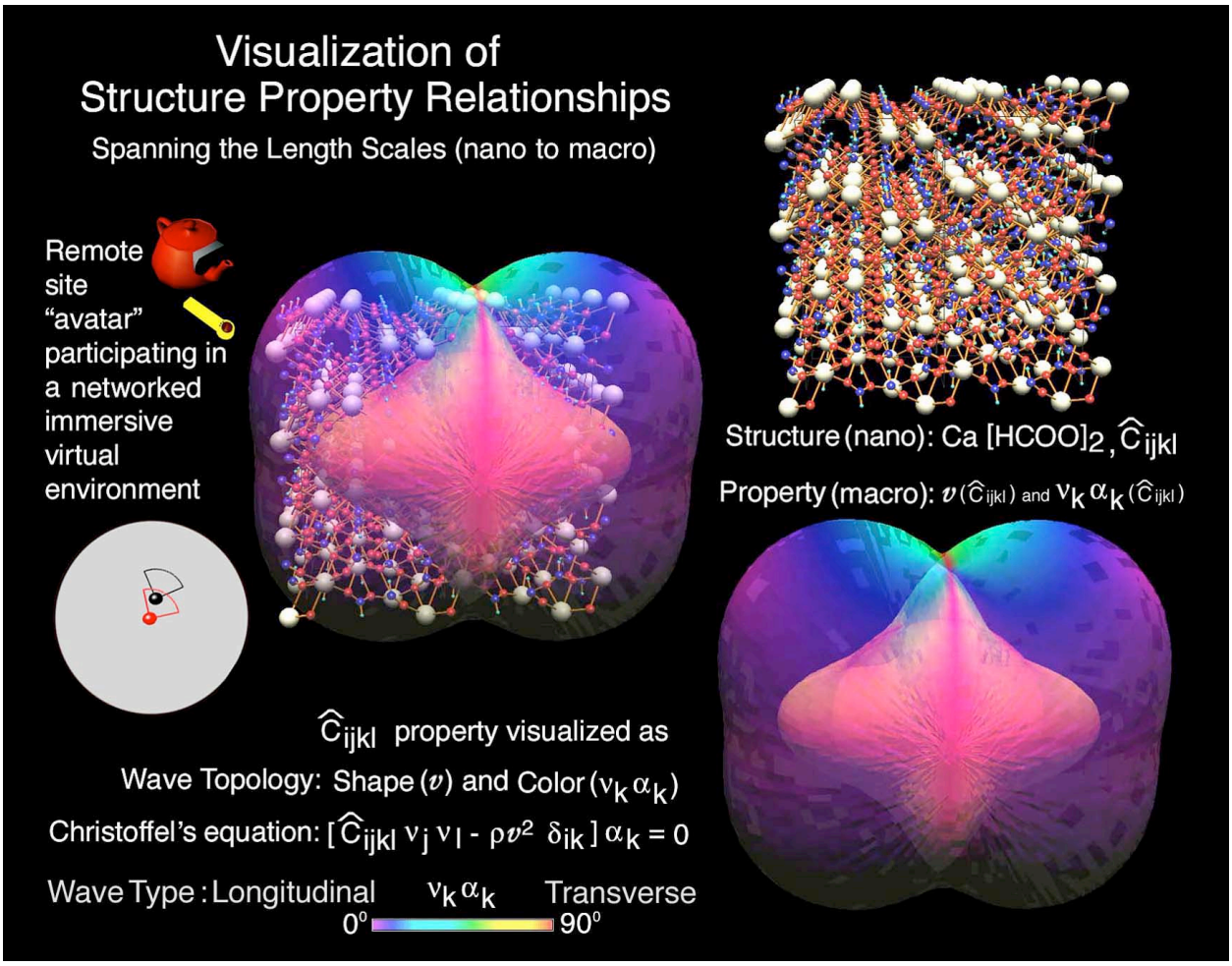

Figure 1b. Description of Nano-Macro Topology for Ca[HCOO]2