The local structure fingerprint of dual orbital degeneracy lifting in a strongly correlated electron system

R. J. Koch[1], R. Sinclair[2], M. T. McDonnell[3], R. Yu[1], M. Abeykoon[4], M. G. Tucker[3], A. M. Tsvelik[1], S. J. L. Billinge[1,5], H. D. Zhou[2], W.-G. Yin[1], E. S. Bozin[1]

[1]Condensed Matter Physics and Materials Science Division, Brookhaven National Laboratory, Upton, NY 11973, US, [2]Department of Physics and Astronomy, University of Tennessee, Knoxville, TN 37996, USA, [3]Neutron Scattering Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA, [4]Photon Sciences Division, Brookhaven National Laboratory, Upton, NY 11973, USA, [5]Department of Applied Physics and Applied Mathematics, Columbia University, New York, NY~10027, USA

rkoch@bnl.gov

The local structure of $NaTiSi_2O_6$ is examined across its Ti-dimerization orbital-assisted Peierls transition at 210 K. An atomic pair distribution function approach evidences local symmetry breaking pre-existing far above the transition. The analysis shows the dimers evolve on heating into a short-range orbital degeneracy lifted (ODL)[1] state of dual orbital character, present up to at least 490 K. The ODL state is correlated over the length scale spanning ~6 sites of the Ti zigzag chains. Our results imply that the ODL phenomenology extends to strongly correlated electron systems.

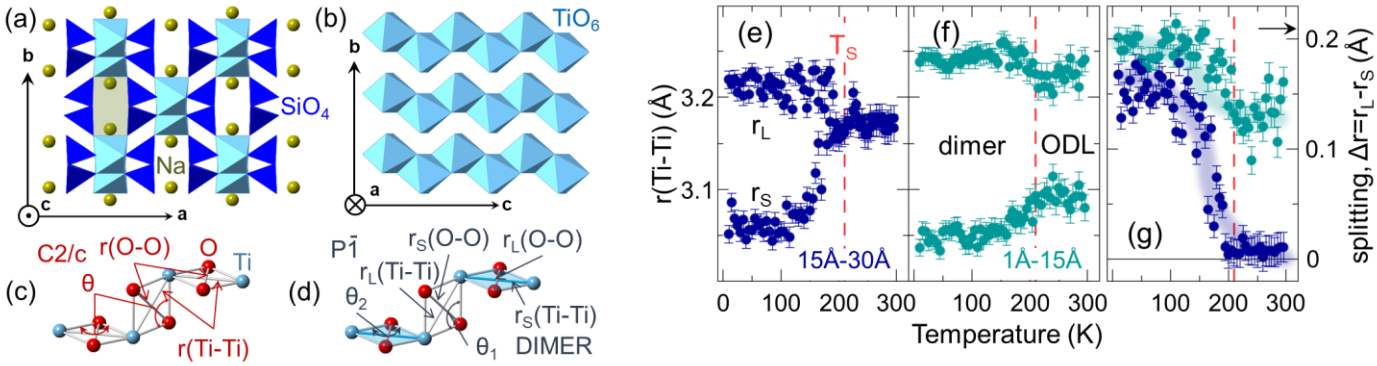

Figure 1. (a) *C*2/*c* structure of $NaTiSi_2O_6$ (b) Quasi-1D zigzag TiO_6 chains; (c) undistorted TiO_2 plaquettes of the *C*2/*c* phase, with uniform Ti-Ti and O-O distances; (d) distorted TiO_2 plaquettes of the dimerized $P\bar{1}$ phase, with Ti-Ti and O-O distances split (S=short, L=long). The nearest neighbour Ti-Ti distances from $P\bar{1}$-based model fits over (e) 15-30 Å and (f) 1-15 Å ranges. The assocaited *r*(Ti-Ti) splitting are shown in (g).

[1] Bozin, E. S., Yin, W. G., Koch, R. J., Abeykoon, M., Hor, Y. S., Zheng, H., Lei, H. C., Petrovic, C., Mitchell, J. F. &. Billinge, S. J. L (2019). *Nat. Comm.* **10**, 3638.

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