

SUPPLEMENTARY MATERIAL

Predicting XAFS scattering path cumulants and XAFS spectra for metals (Cu, Ni, Fe, Ti, Au) using molecular dynamics simulations

M.A. Karolewski^{1,*}, R.G. Cavell¹, R.A. Gordon², C.J. Glover³, M. Cheah³, and M.C. Ridgway⁴.

¹ Department of Chemistry, University of Alberta, Edmonton, Alberta T6G 2G2, Canada.

² Pacific Northwest Consortium Synchrotron Radiation Facility, APS Sector 20, 9700 S. Cass Ave. Bldg. 435E, Argonne, IL, USA 60439.

³ Australian Synchrotron, Clayton, VIC 3168, Australia.

⁴ Department of Electronic Materials Engineering, Research School of Physics and Engineering, Australian National University, ACT 0200, Australia.

* Corresponding author. E-mail address: karolewski@alum.mit.edu.

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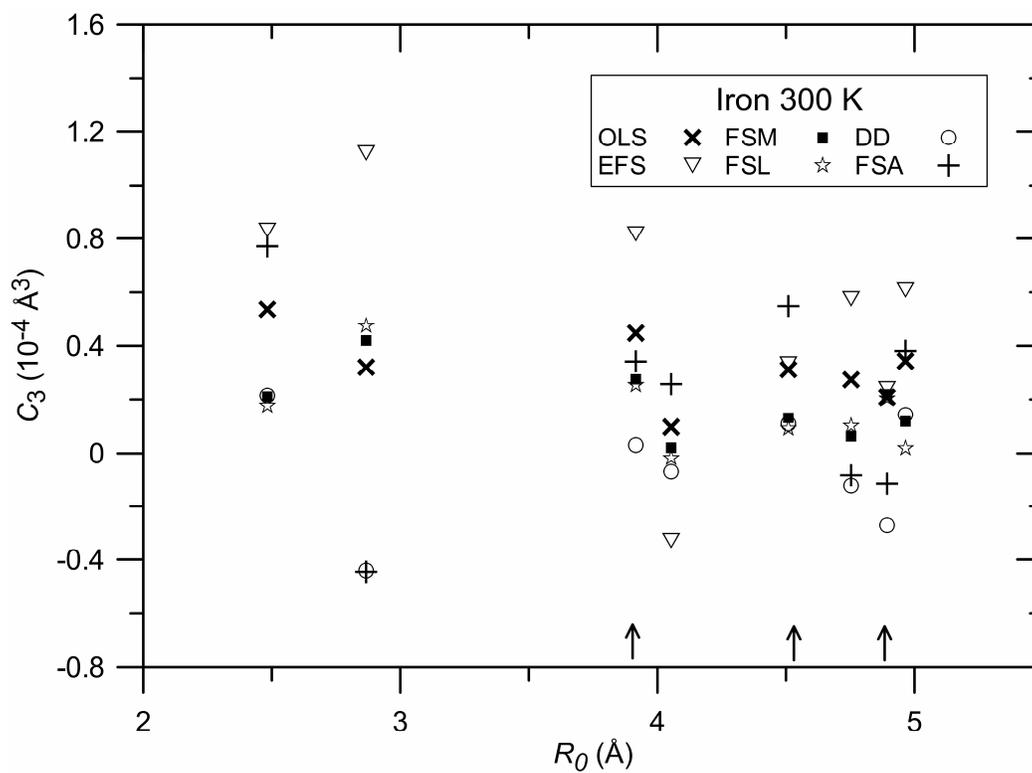


Figure S2. Third cumulants (C_3) for several XAFS scattering paths predicted by MD simulations for Fe at 300 K. Data for multiple-scattering paths are indicated by arrows.

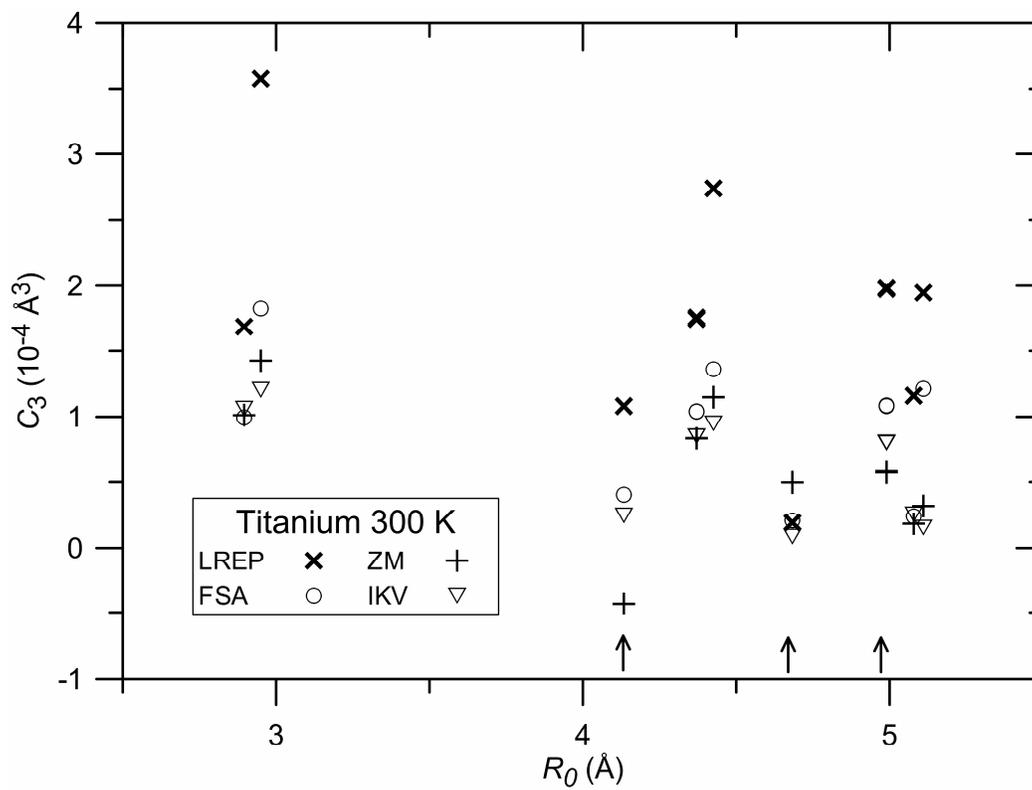


Figure S3. Third cumulants (C_3) for several XAFS scattering paths predicted by MD simulations for Ti at 300 K. Data for multiple-scattering paths are indicated by arrows.

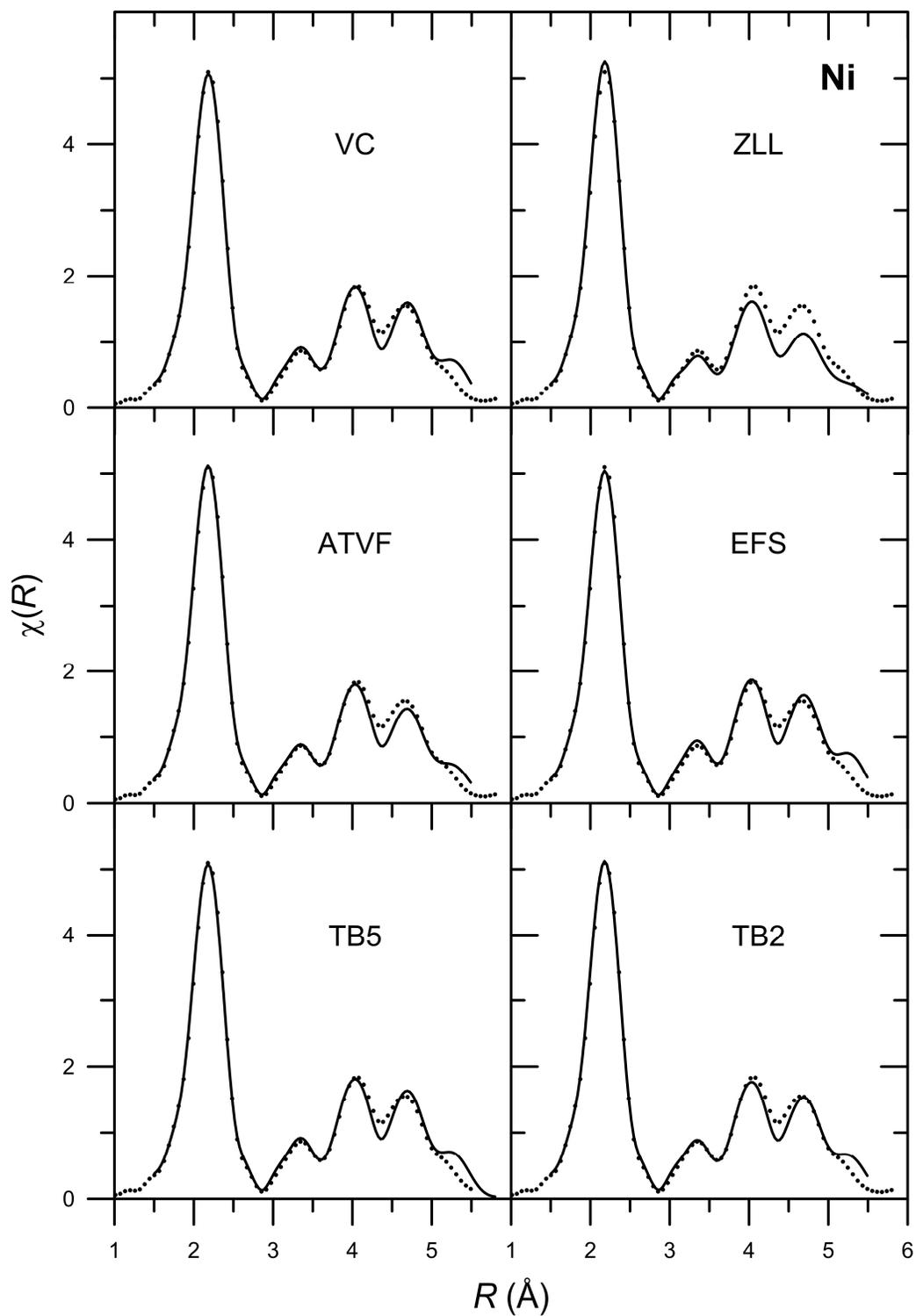


Figure S4. Symbols: experimental XAFS spectrum for Ni; solid lines: XAFS spectra fitted using scaled MD cumulants (solid lines; see main text for fitting details).

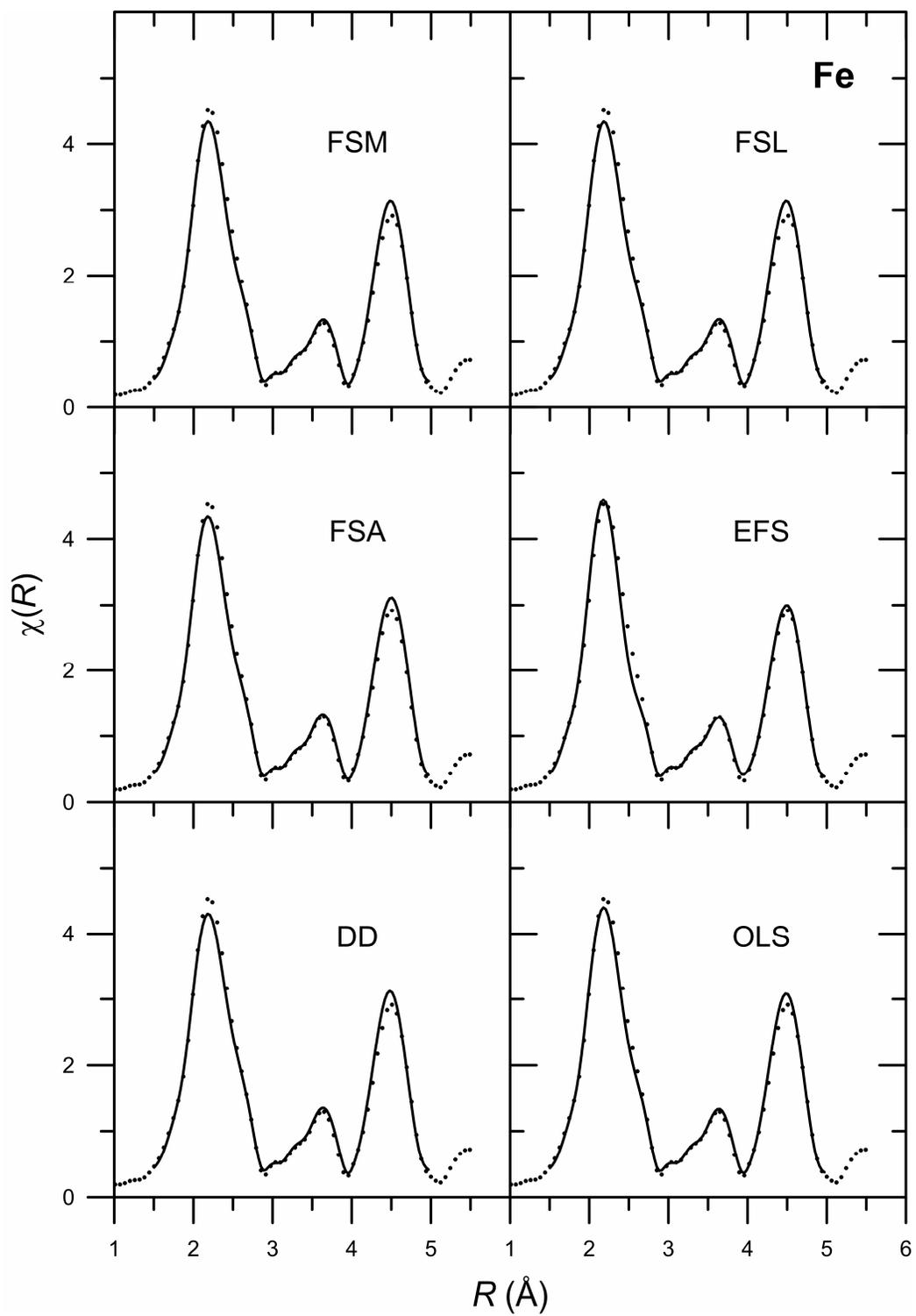


Figure S5. Symbols: experimental XAFS spectrum for Fe; solid lines: XAFS spectra fitted using scaled MD cumulants (solid lines; see main text for fitting details).

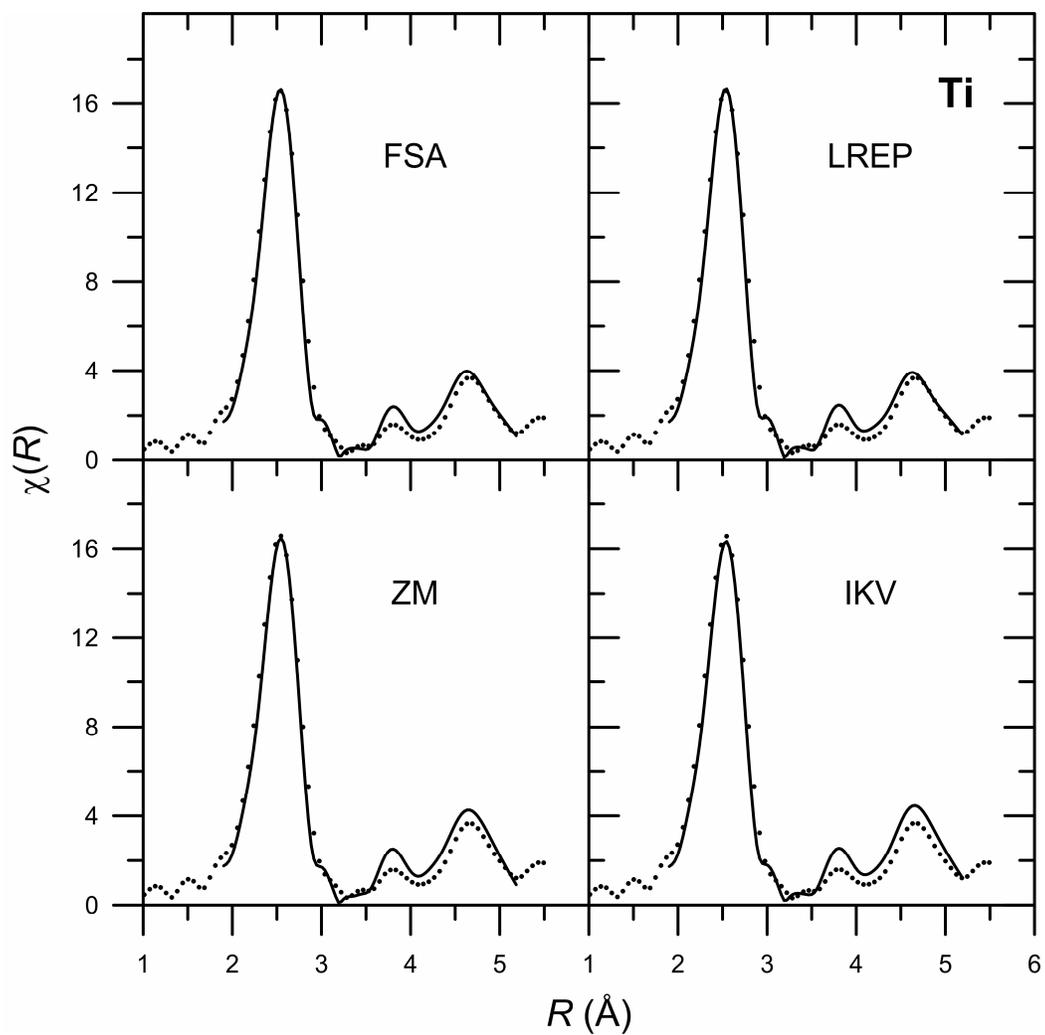


Figure S6. Symbols: experimental XAFS spectrum for Ti; solid lines: XAFS spectra fitted using scaled MD cumulants (solid lines; see main text for fitting details).

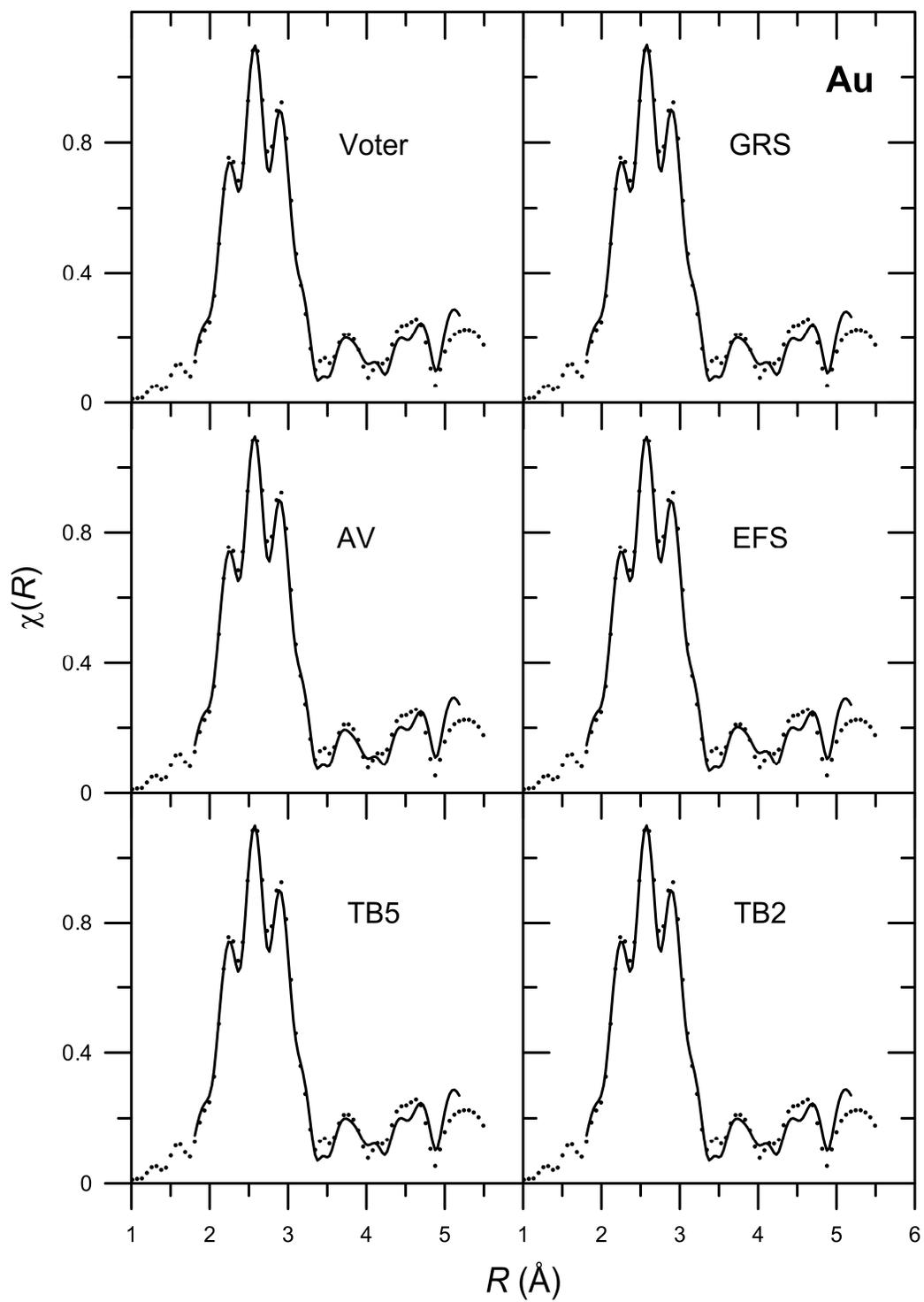


Figure S7. Symbols: experimental XAFS spectrum for Au; solid lines: XAFS spectra fitted using scaled MD cumulants (solid lines; see main text for fitting details).