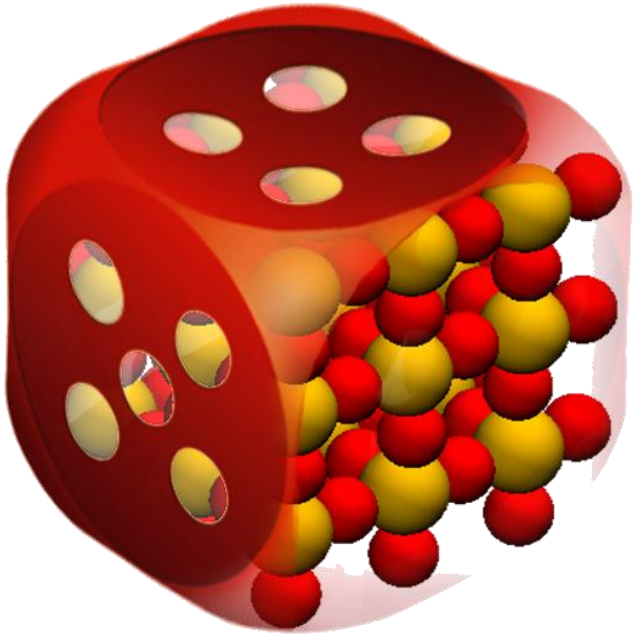
The 15th International Conference on X-ray Absorption Fine Structure



An efficient implementation of the reverse Monte Carlo method for EXAFS analysis in crystalline materials

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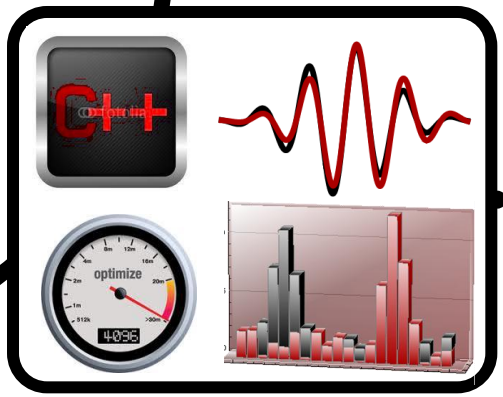
Latvian Government Research Grant No. 09.1518.

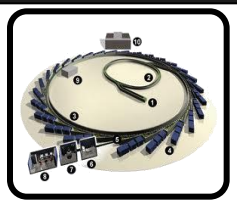
High-quality experimental data (synchrotron radiation source)

High-performance computing systems

EXAFS-RMC



Ab-initio *EXAFS calculations (*FEFF *code)*
Software development & optimization
Data analysis

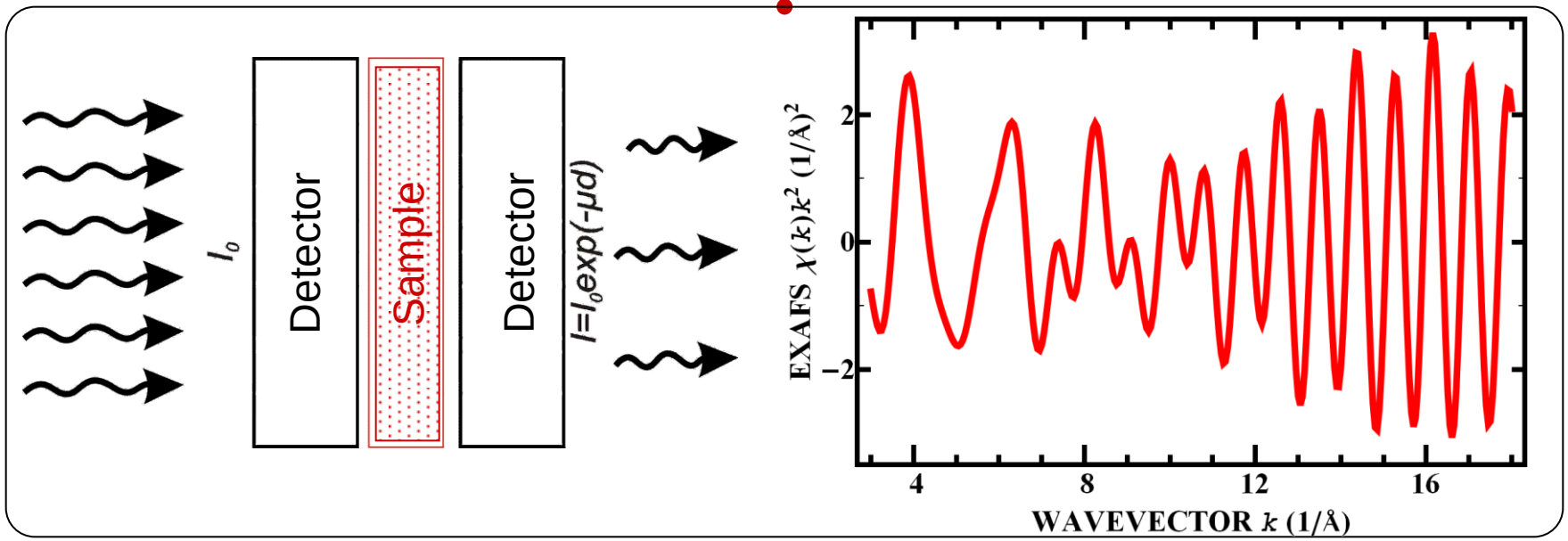


Experimental data:
EXAFS spectroscopy

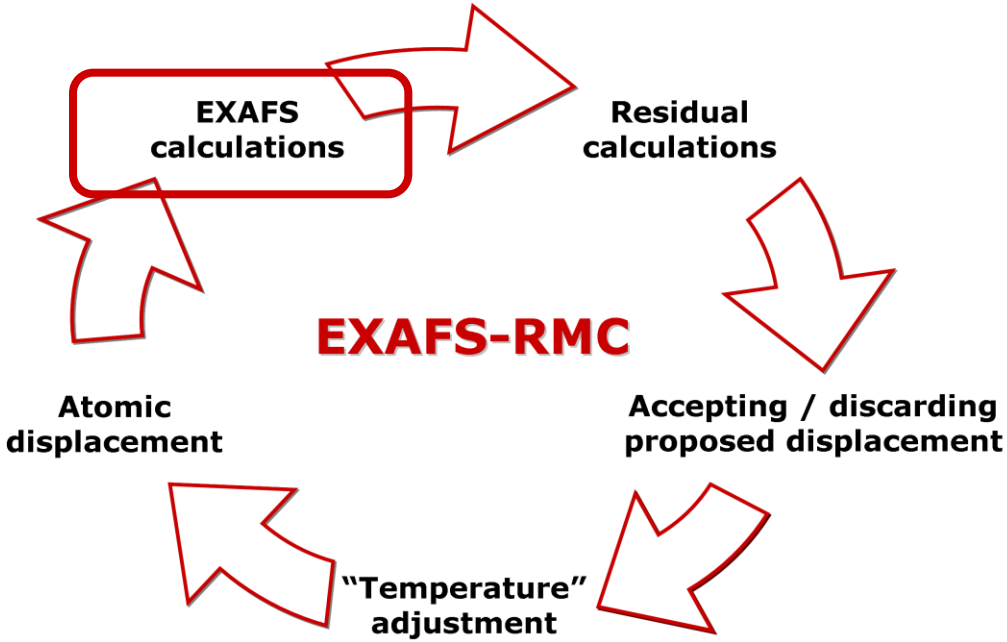
$$\chi(k) = \sum_p g_p(r_{p1}, r_{p2}, \ldots) A_p(k, r_{p1}, r_{p2}, \ldots) \sin\left(2kR_p + \phi_p(k, r_{p1}, r_{p2}, \ldots)\right)$$

Experiment — **RMC** — **FEFF**

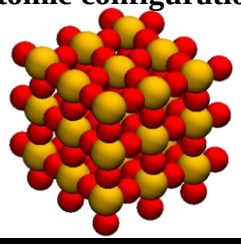
Ankudinov A, Ravel B, Rehr J and Conradson S
1998 Phys. Rev. B 58 7565



Reverse Monte Carlo: algorithm

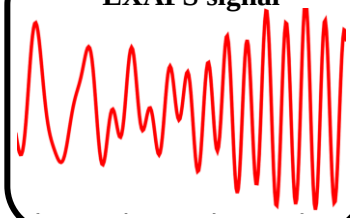


Atomic configurations



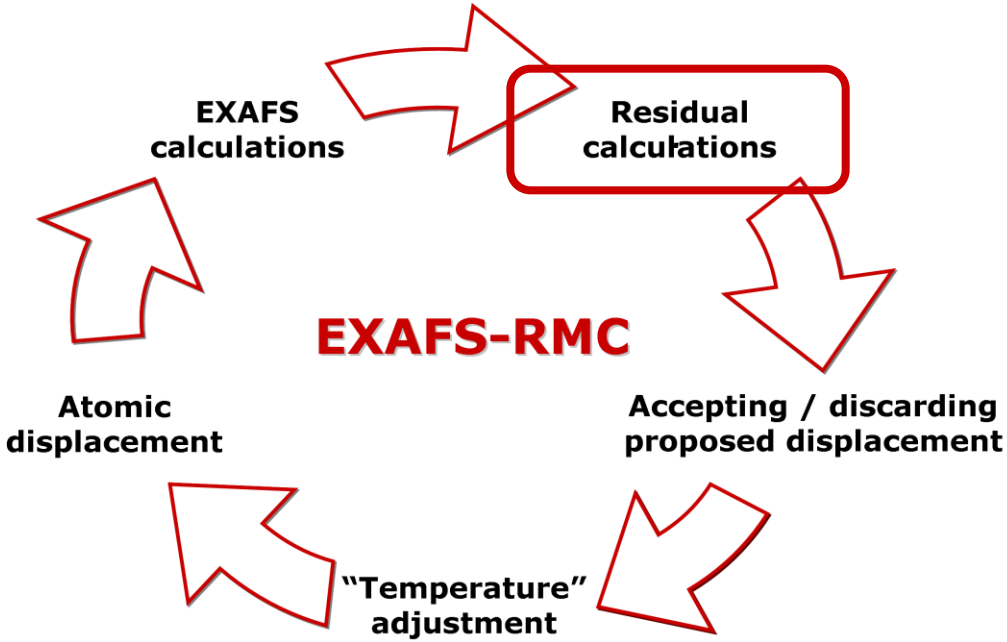
Ab-initio multiple-scattering EXAFS calculations for given atomic configuration by FEFF8 code

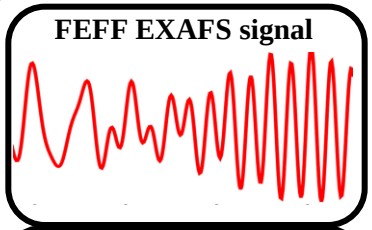
EXAFS signal

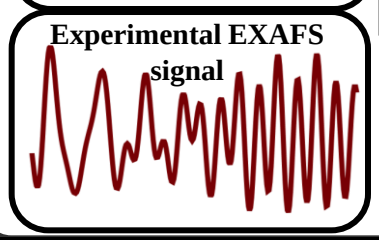


J.Timoshenko, A. Kuzmin, J. Purans, Comp. Phys. Commun. 2012
A. L. Ankudinov, B. Ravel, J. J. Rehr, S. D. Conradson, Phys. Rev. B 1998

Reverse Monte Carlo: algorithm

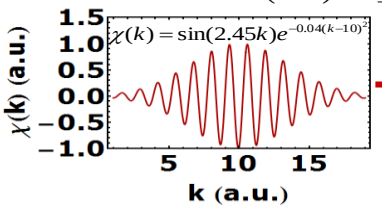


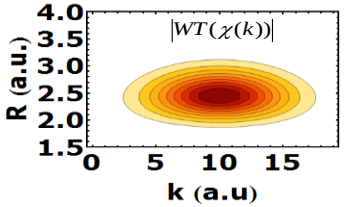




Wavelet transform:

$$WT(k,R) = \left(\frac{2R}{c}\right)^{0.25} \int_{-\infty}^{\infty} \chi(k) e^{-2iR(k'-k)} e^{-\frac{2R}{c}(k'-k)^2} dk'$$



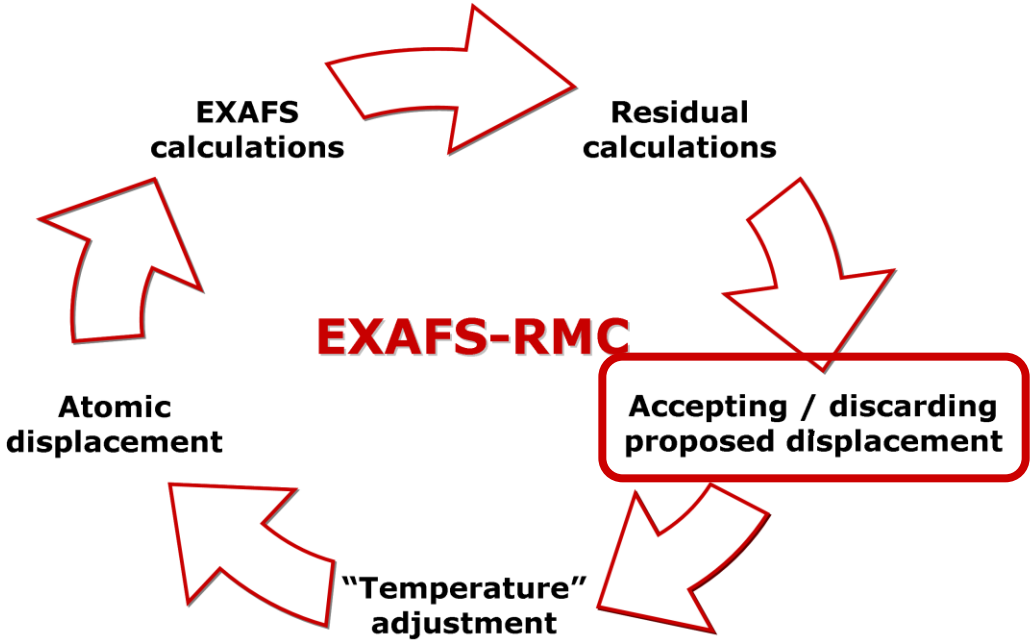


Residual

$$\varepsilon = |WT_{exp} - WT_{FEFF}|$$

J. Timoshenko, A. Kuzmin, Comp. Phys. Commun. 2009

Reverse Monte Carlo: algorithm



Metropolis algorithm:

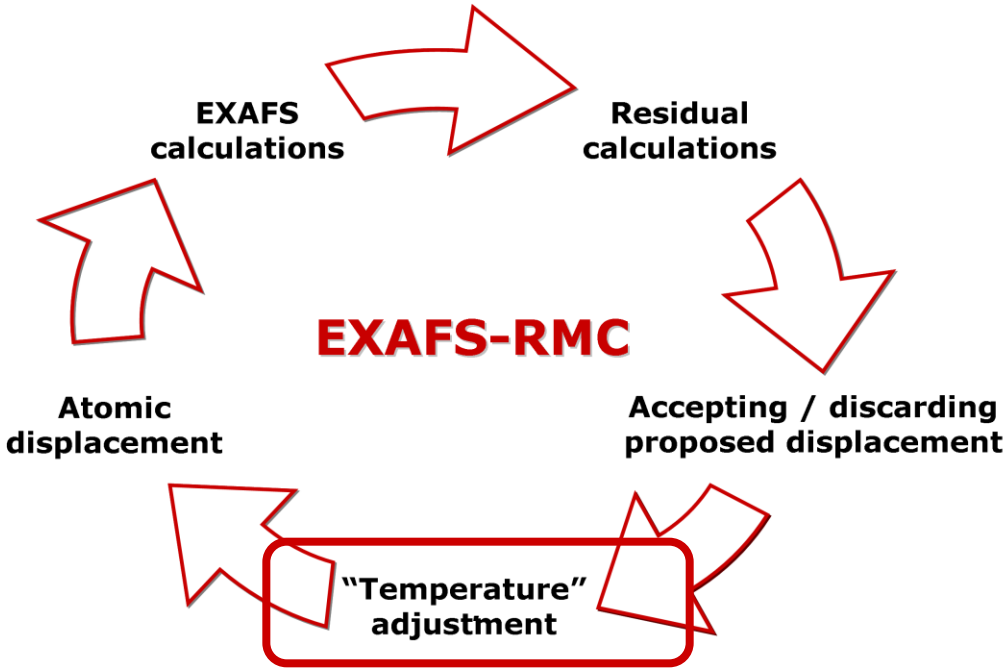
- $\varepsilon < \varepsilon_{old}$: move is accepted
- $\varepsilon > \varepsilon_{old}$: move is accepted, if

$$\exp[-(\varepsilon - \varepsilon_{old}) / T] > \textit{random number}$$

***T* – scaling parameter, "temperature"**

N. Metropolis, A. W. Rosenbluth, M. N. Rosenbluth, A. H. Teller, E. Teller, J Chem. Phys. 1953

Reverse Monte Carlo: algorithm



Simulated annealing:

$T = -\Delta(t) / \ln[1 - p(t)]$

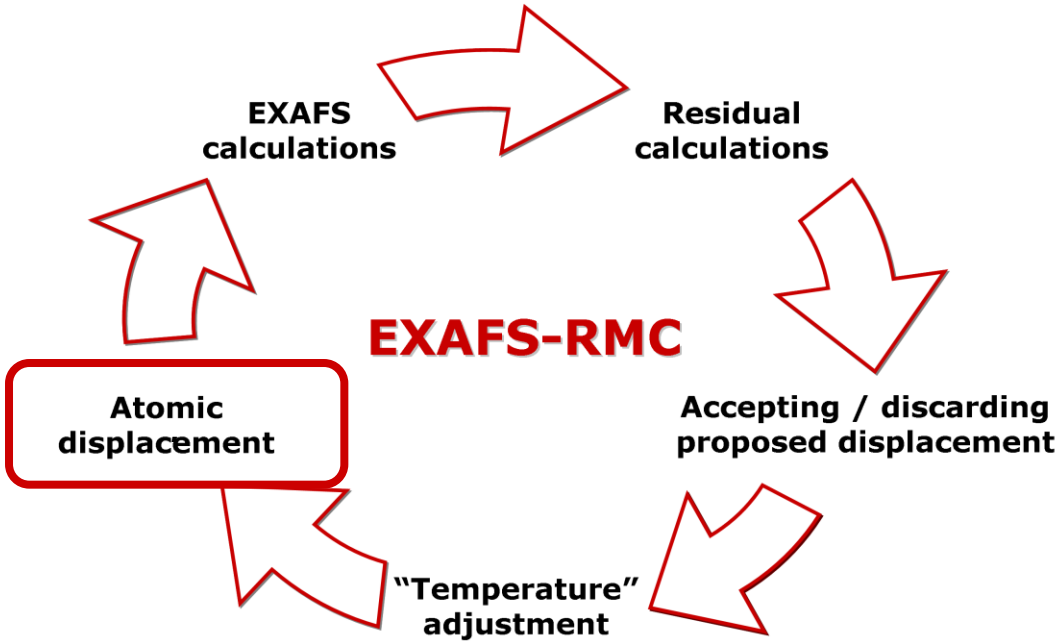
$p(t) = t / t_{max}$ – target value for moves discarding rate;

$\Delta(t)$ – average residual change per one move

J.Timoshenko, A. Kuzmin, J. Purans, Comp. Phys. Commun. 2012

S. Kirkpatrick, C. D. Gelatt, M. P. Vecchi, Science 1983

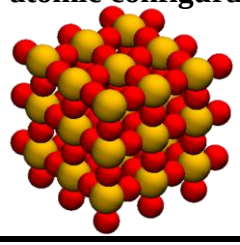
Reverse Monte Carlo: algorithm



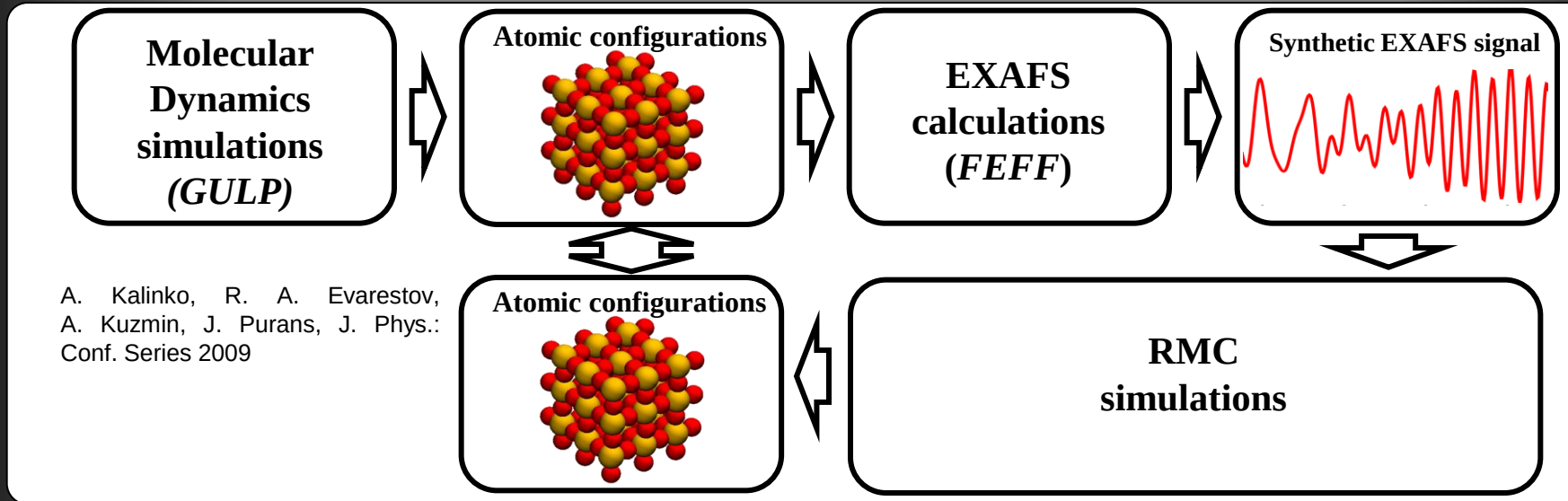
Coordinates of all particles are slightly, randomly changed:

$$\vec{r}_i(t+\Delta t) = \vec{r}_i(t) + \vec{\delta}_i$$

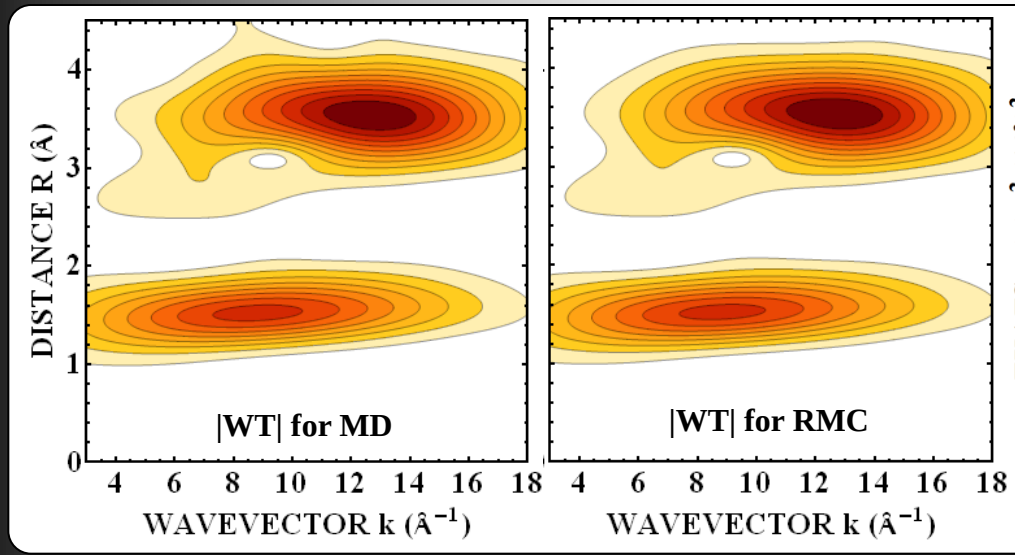
New atomic configuration

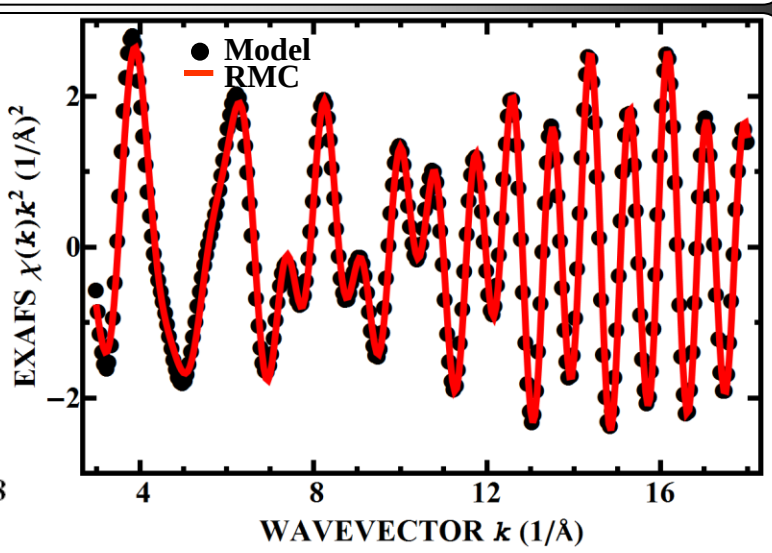


Testing method: synthetic data

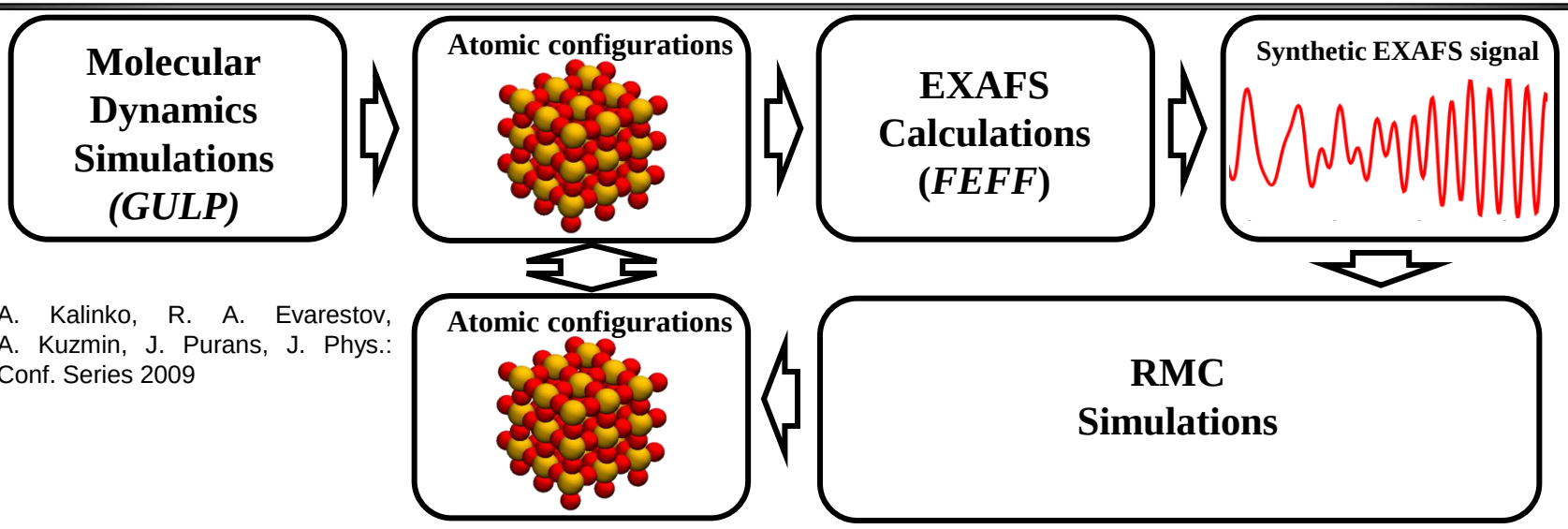


A. Kalinko, R. A. Evarestov, A. Kuzmin, J. Purans, J. Phys.: Conf. Series 2009

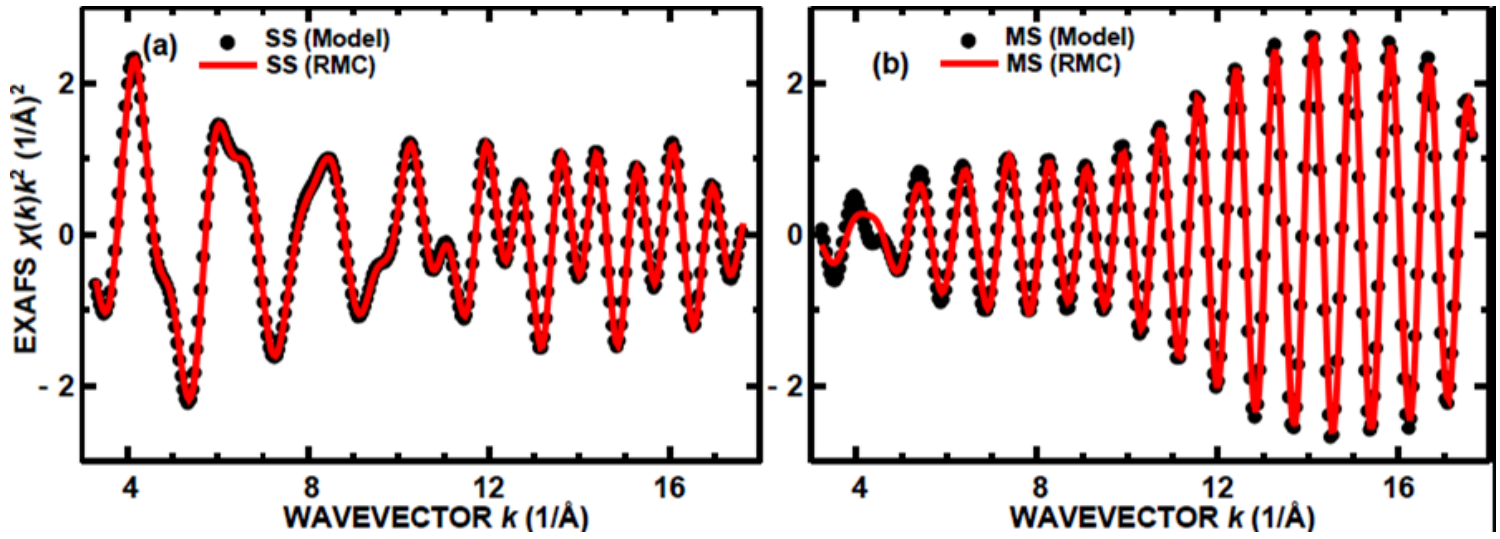




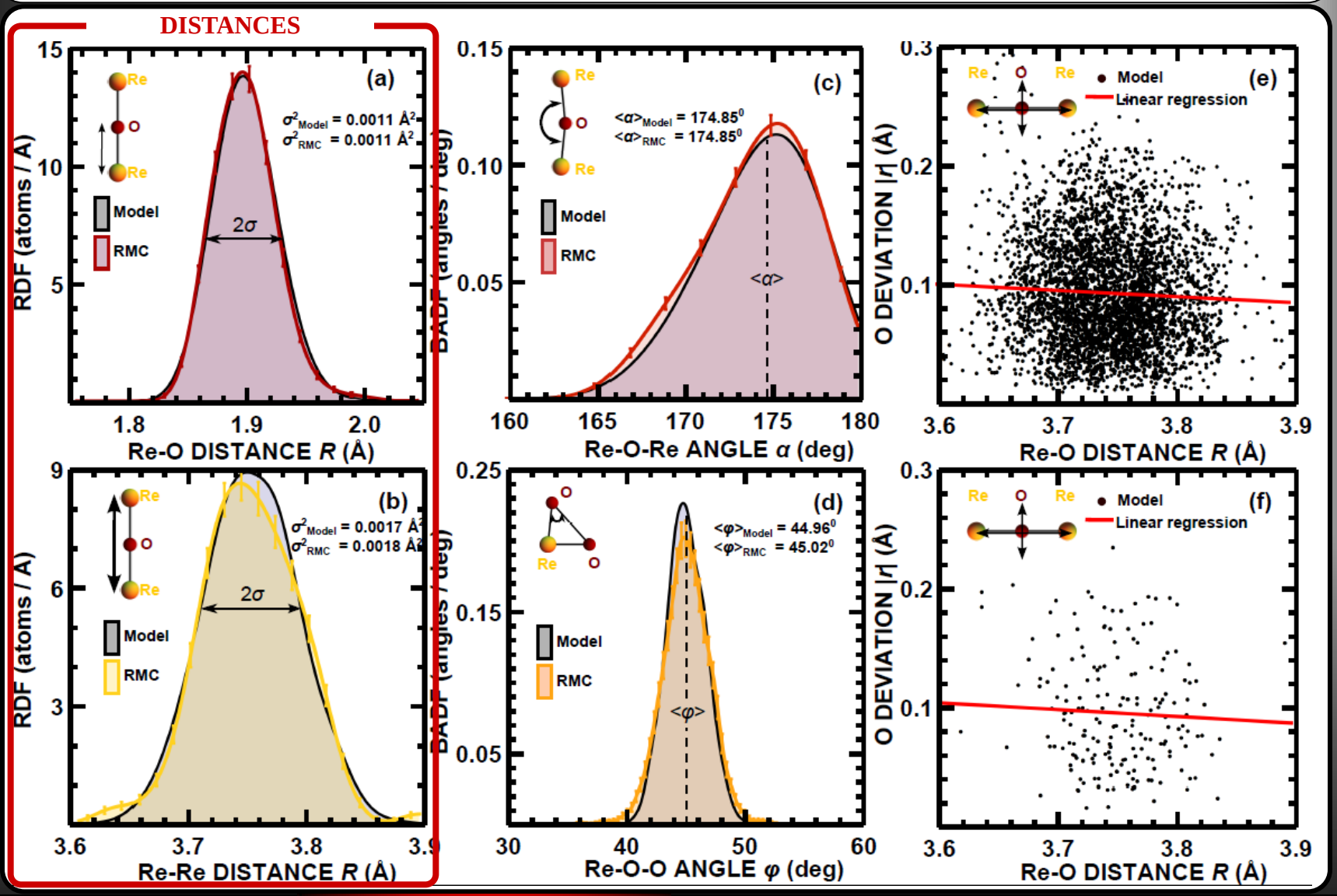
Testing method:
synthetic data



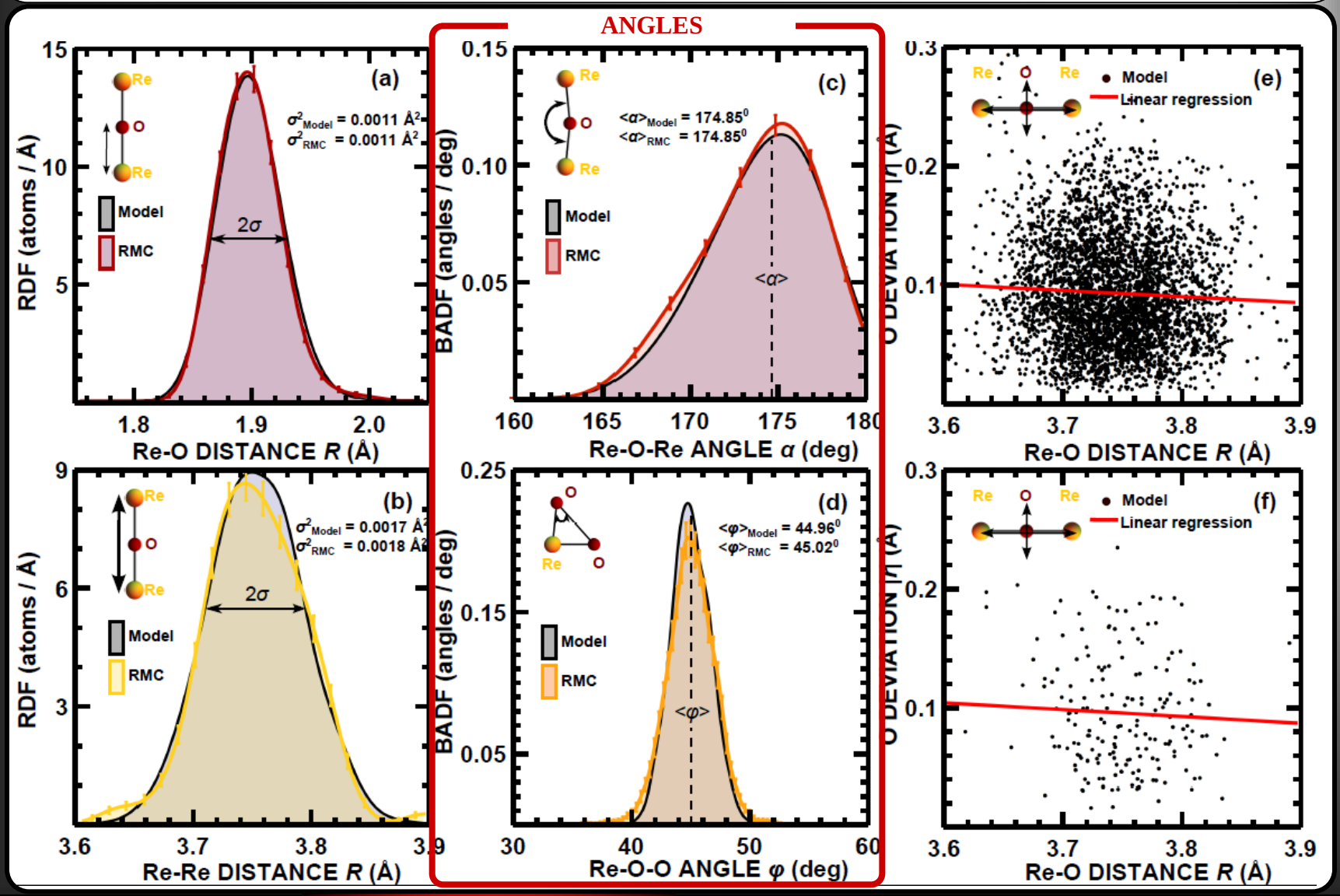
A. Kalinko, R. A. Evarestov, A. Kuzmin, J. Purans, J. Phys.: Conf. Series 2009



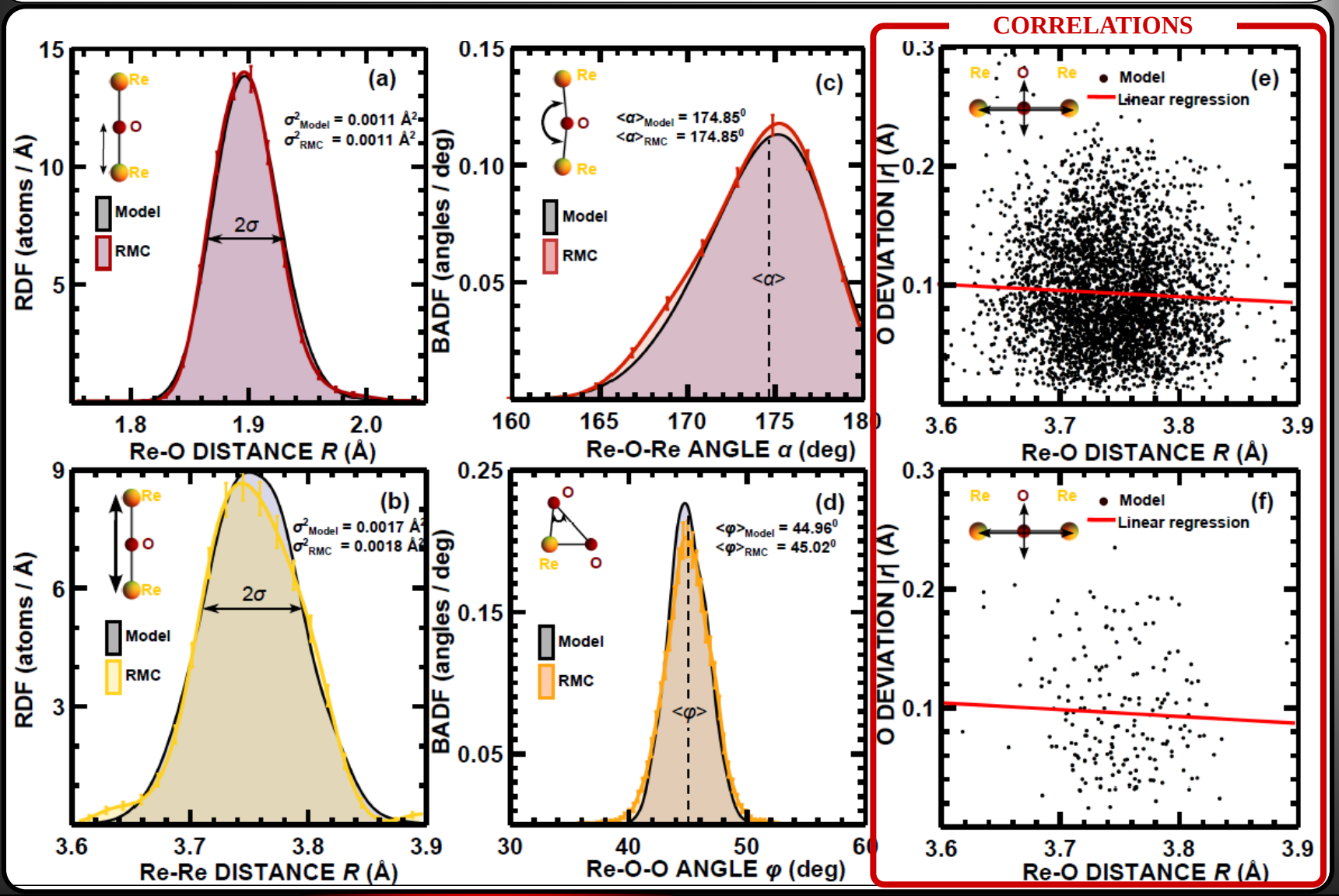
Testing method: results

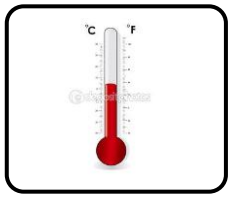


Testing method: results

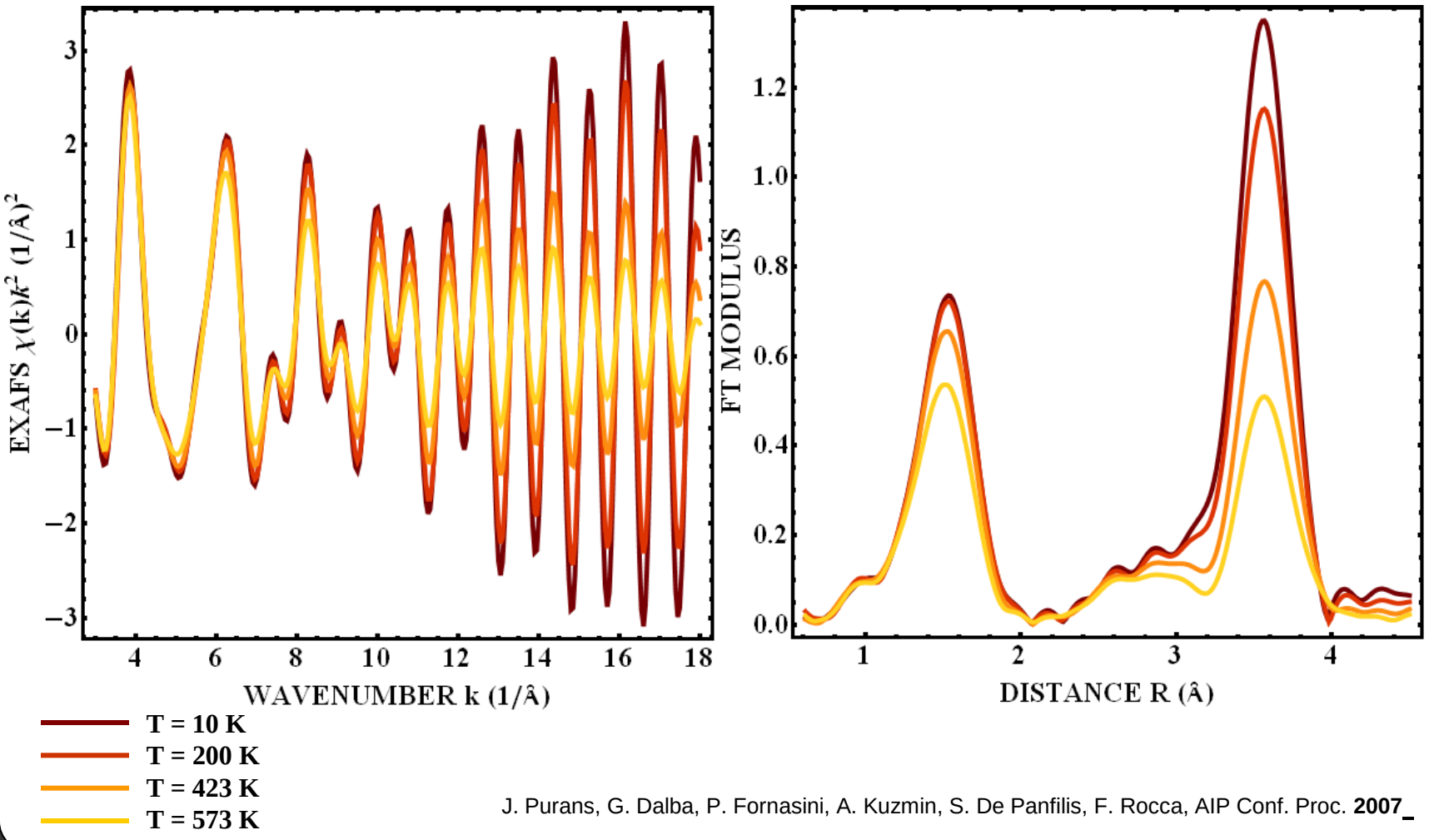


Testing method: results

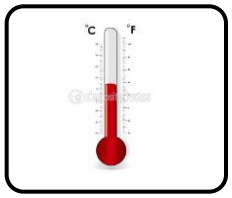




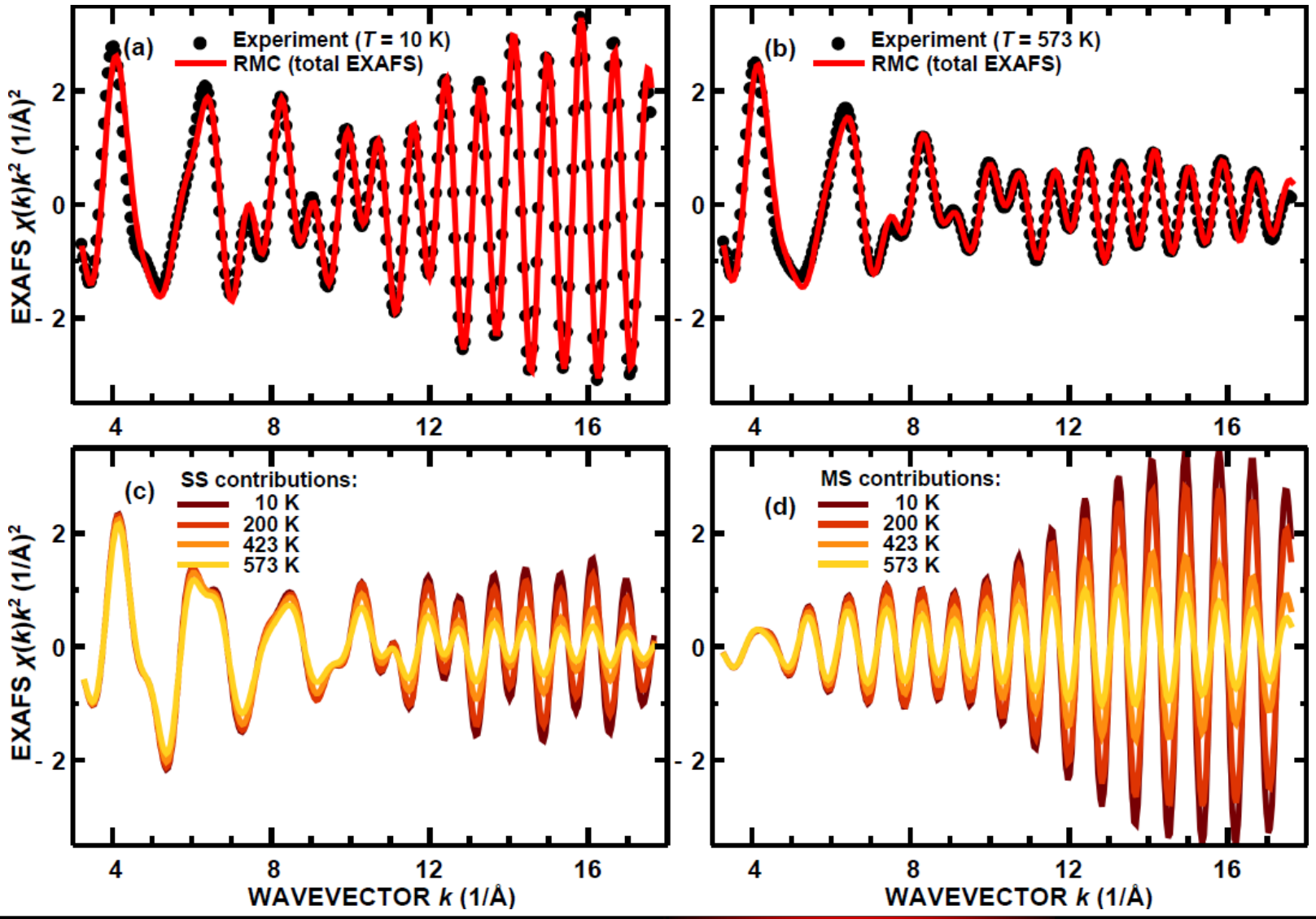
Thermal disorder in ReO_3: experimental EXAFS data

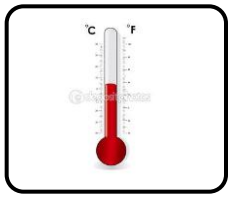


J. Purans, G. Dalba, P. Fornasini, A. Kuzmin, S. De Panfilis, F. Rocca, AIP Conf. Proc. **2007**_

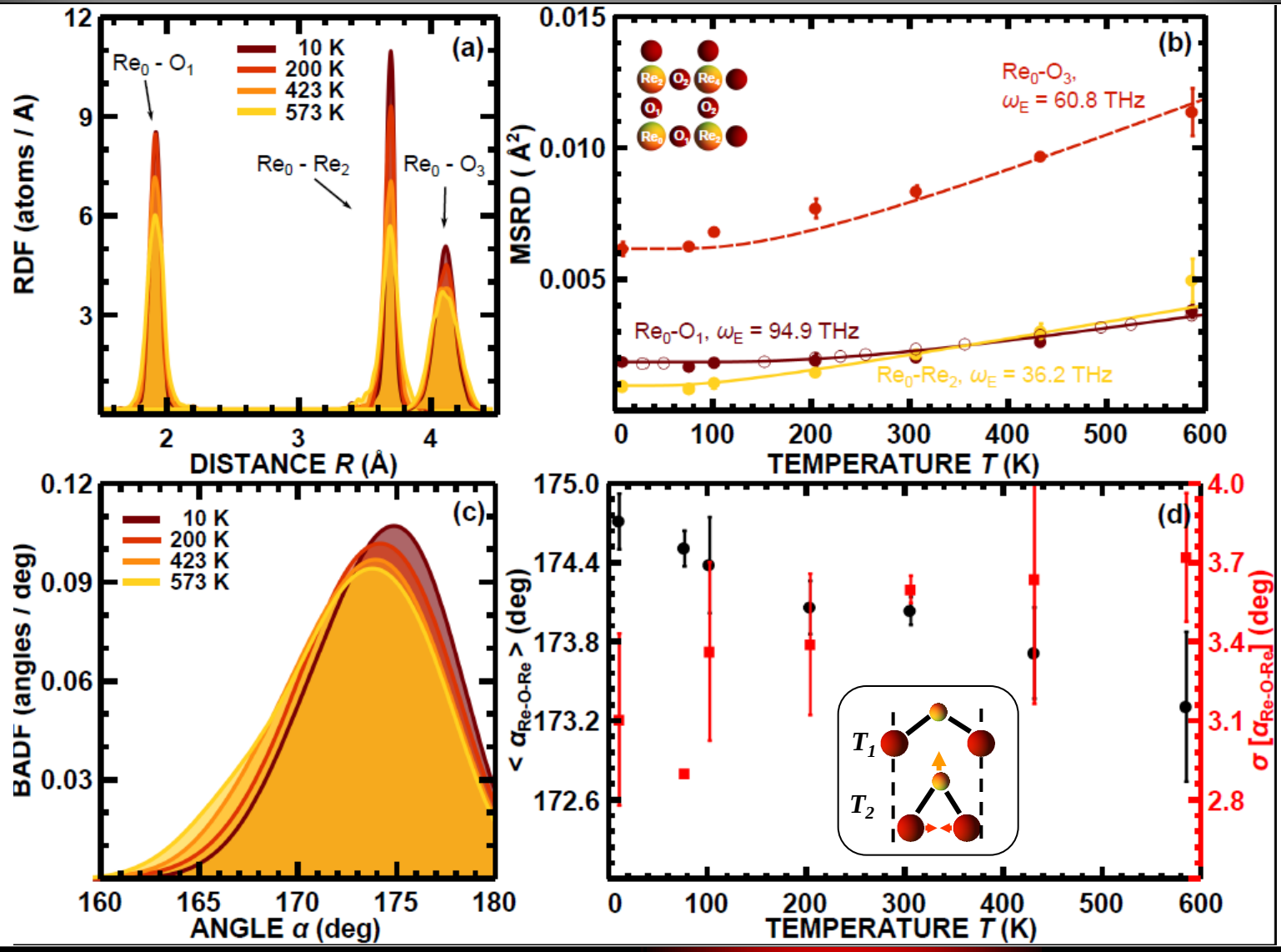


Thermal disorder in ReO_3: RMC fits; SS and MS contributions





Thermal disorder in ReO_3: Interatomic distances



Summary

- Reverse Monte Carlo method can be successfully used to interpret EXAFS spectra of crystalline materials even in case, when the multiple-scattering effects are very pronounced.

- For the first time the analysis of the Re L_3-edge EXAFS data from the second and third coordination shells of rhenium in ReO_3 has been carried out.

- The obtained results are in agreement with the rigid unit model of lattice dynamics in ReO_3: displacements of oxygen and nearest rhenium atoms, and oxygen motion in the direction orthogonal to the Re_0-Re_2 bond and the average Re_0-Re_2 distance are strongly correlated.

Thank you for your attention!..