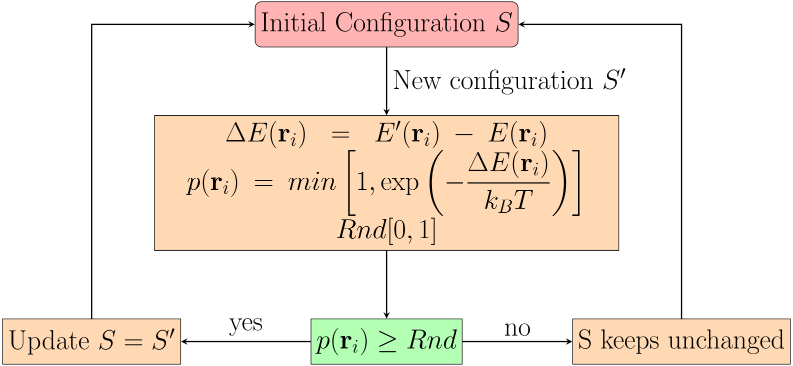
# Canonical Monte Carlo

## Metropolis algorithm

Temperature=const., $E = E_D + E_{dip} + E_{gr} + E_e$




Model for relaxor: Ma, Albe, and Xu, Phys. Rev. B 91, 184108 (2015)

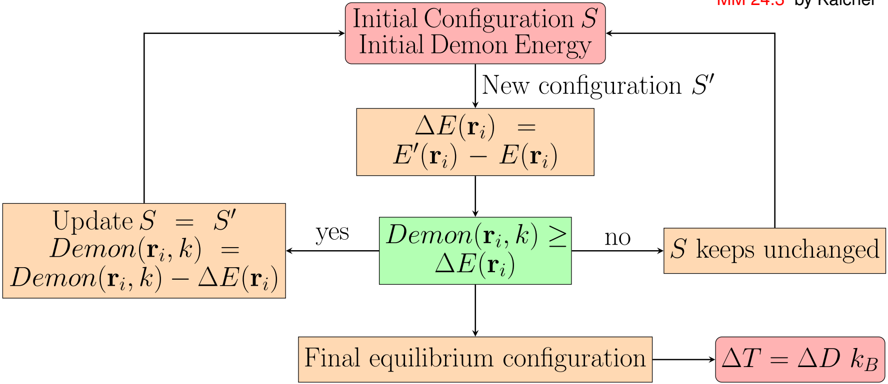
# Micrcanonical Monte Carlo

## Multi-demon algorithm



Total energy=const., $E^* = E_D + E_{dip} + E_{gr} + E_e + E_k$

SYCE 1.3 by Grünebohm
MM 24.3 by Kalcher




Ponomareva & Lisenkov, Phys. Rev. Lett. (2012).

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# Lattice-based Monte Carlo

## Energy terms

$$E = E_D + E_{dip} + E_{gr} + E_e$$

- Landau potential

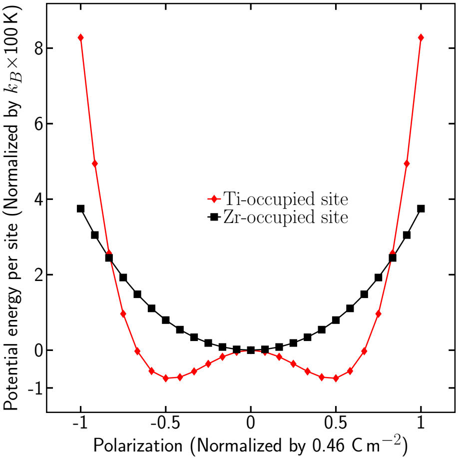
$$E_D = V_0 \sum_i \left[ \frac{a_i}{2}(P_x^2(\mathbf{r}_i) + P_y^2(\mathbf{r}_i)) + \frac{b_i}{4}(P_x^4(\mathbf{r}_i) + P_y^4(\mathbf{r}_i)) + \frac{c_i}{6}(P_x^6(\mathbf{r}_i) + P_y^6(\mathbf{r}_i)) \right]$$

$$\begin{cases} a_i = -13.7128 \times 10^8\,\mathrm{J\,m\,C^{-2}},\ b_i = 28.908 \times 10^9\,\mathrm{J\,m^5\,C^{-4}} & \text{(Ti-occupied site)} \\ a_i = 6.112 \times 10^8\,\mathrm{J\,m\,C^{-2}},\ b_i = 1.4454 \times 10^9\,\mathrm{J\,m^5\,C^{-4}} & \text{(Zr-occupied site)} \end{cases}$$

King-Smith & Vanderbilt, Phys. Rev. B (1994)

# Simulation concept

## Behavior of $Ba(Zr_xTi_{1-x})O_3$




King-Smith & Vanderbilt, Phys. Rev. B (1994)

# Lattice-based Monte Carlo

## Energy terms

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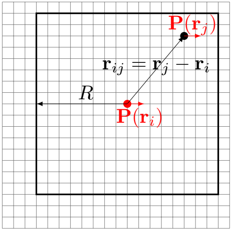
$$E = E_D + E_{dip} + E_{gr} + E_e$$

- Dipole-dipole interaction

$$E_{dip} = V_0^2 \frac{1}{8\pi\epsilon_0} \sum_{i,j} \frac{1}{\epsilon_{ij}} \left[ \frac{\mathbf{P}(\mathbf{r}_i) \cdot \mathbf{P}(\mathbf{r}_j)}{|\mathbf{r}_i - \mathbf{r}_j|^3} - \frac{3[\mathbf{P}(\mathbf{r}_i) \cdot (\mathbf{r}_i - \mathbf{r}_j)][\mathbf{P}(\mathbf{r}_j) \cdot (\mathbf{r}_i - \mathbf{r}_j)]}{|\mathbf{r}_i - \mathbf{r}_j|^5} \right], \quad (1)$$





Servoin et al., Phys. Rev. B (1980).
Hlinka & Márton, Phys. Rev. B (2006).
Nayak et al., RSC Adv. (2014).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# Lattice-based Monte Carlo

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$$\begin{aligned} E_{dip} &= V_0^2 \frac{1}{8\pi\epsilon_0} \sum_{i,j} \frac{1}{\epsilon_{ij}} \left[ \frac{\mathbf{P}(\mathbf{r}_i) \cdot \mathbf{P}(\mathbf{r}_j)}{|\mathbf{r}_i - \mathbf{r}_j|^3} \right. \\ &- \left. \frac{3[\mathbf{P}(\mathbf{r}_i) \cdot (\mathbf{r}_i - \mathbf{r}_j)][\mathbf{P}(\mathbf{r}_j) \cdot (\mathbf{r}_i - \mathbf{r}_j)]}{|\mathbf{r}_i - \mathbf{r}_j|^5} \right], \end{aligned}$$

$$\epsilon_{ij} = \begin{cases} 12.0 & \text{both sites } i \ \& \ j \text{ are occupied by Ti,} \\ 144.0 & \text{both sites } i \ \& \ j \text{ are occupied by Zr,} \\ 12.0(1-x) + 144.0x & \text{if site } i \ \& \ j \text{ are occupied by Ti and Zr, respectively.} \end{cases}$$

where x is the Zr-content.

Servoin et al., Phys. Rev. B (1980).
Hlinka & Márton, Phys. Rev. B (2006).
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