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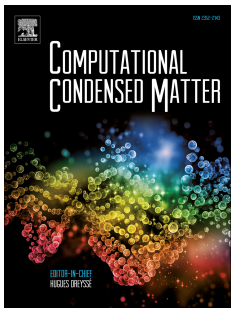

Determination of the lattice thermal conductivity of the TiO_2 polymorphs rutile and anatase by molecular dynamics simulation

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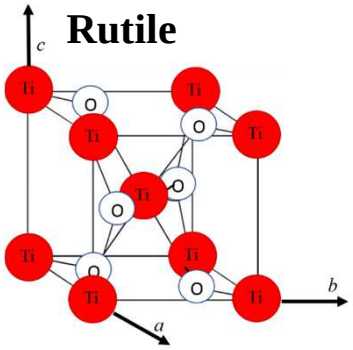
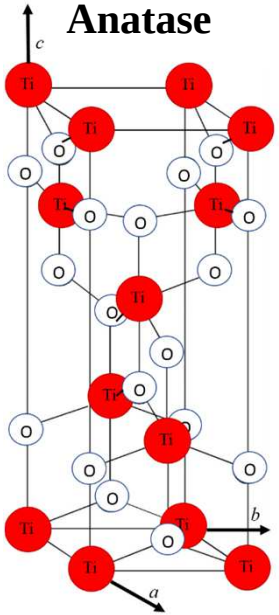
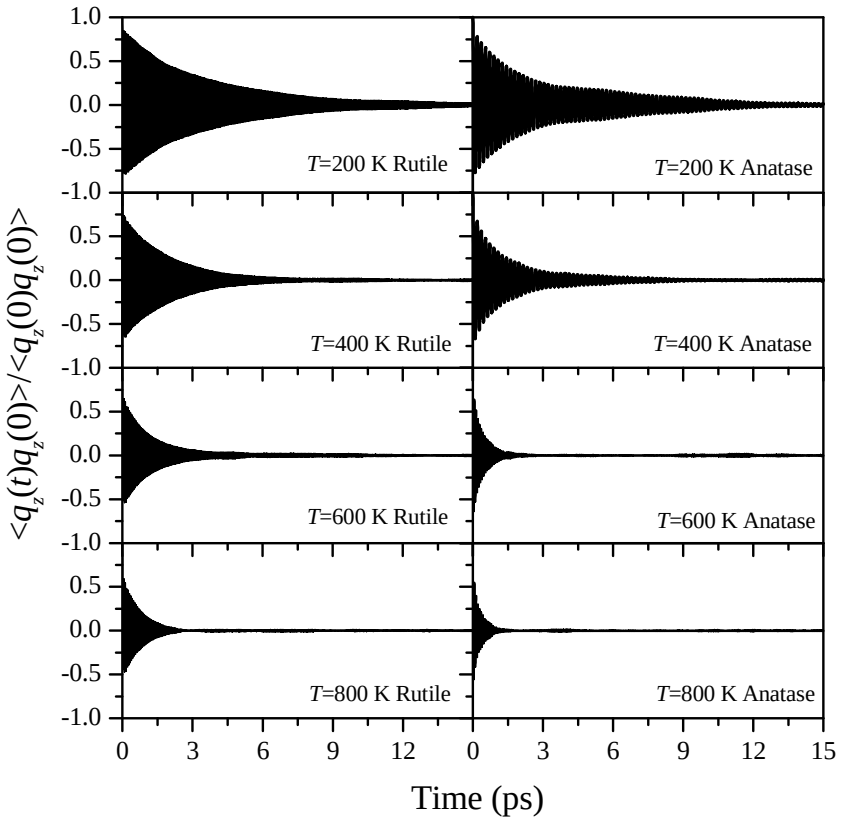
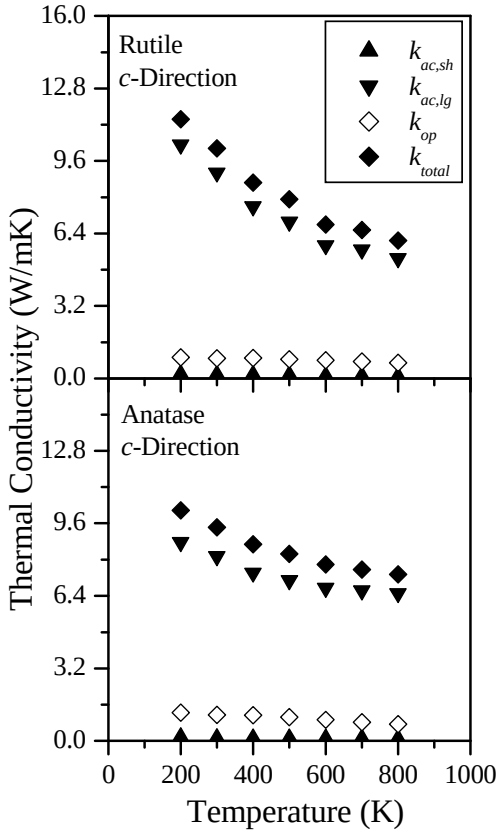

Rutile
c
b
a
Ti
O


Anatase
c
b
a
Ti
O


T=200 K Rutile
T=200 K Anatase
T=400 K Rutile
T=400 K Anatase
T=600 K Rutile
T=600 K Anatase
T=800 K Rutile
T=800 K Anatase
<$q_z(t)q_z(0)$>/<$q_z(0)q_z(0)$>
Time (ps)


Rutile
c-Direction
Anatase
c-Direction
$k_{ac,sh}$
$k_{ac,lg}$
k_{op}
k_{total}
Thermal Conductivity (W/mK)
Temperature (K)

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