Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary material for "Infrared spectroscopy of CeO_2 nanoparticles using Bergman's spectral representation: effects of phonon confinement and lattice strain"

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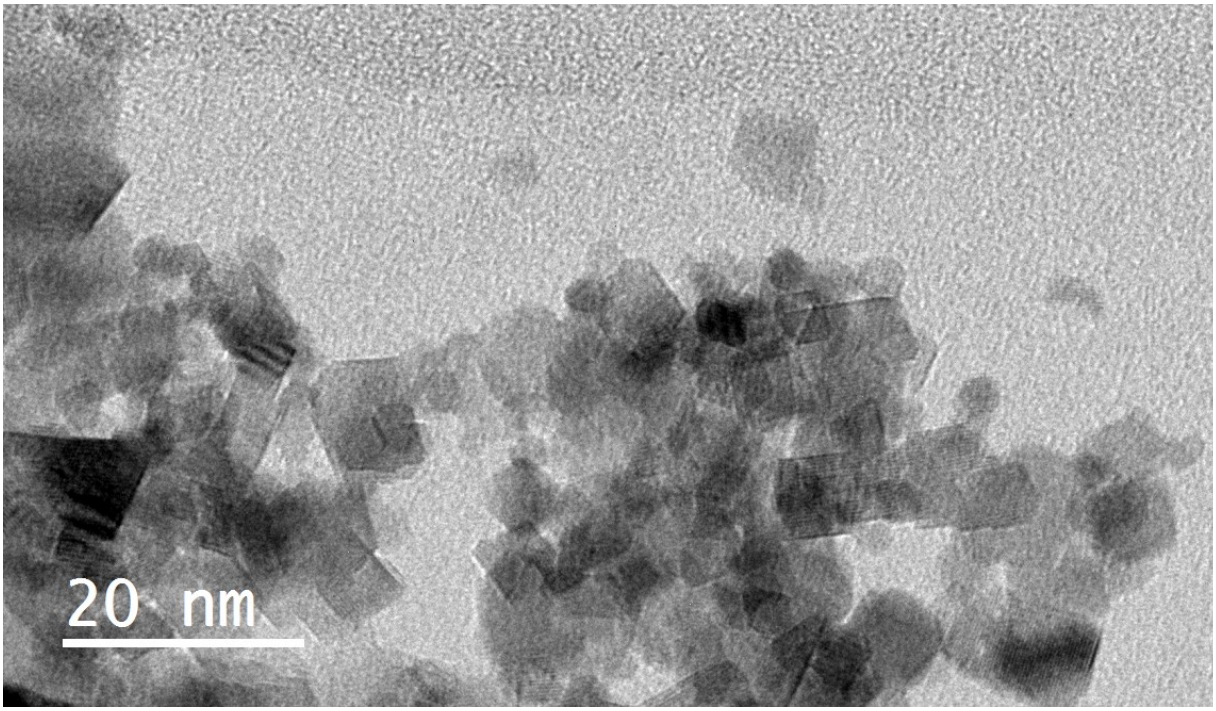

Fig. S1. Close-up HRTEM micrograph of the CeO2 nanoparticles. Atomic diffraction planes can be seen for some particles.

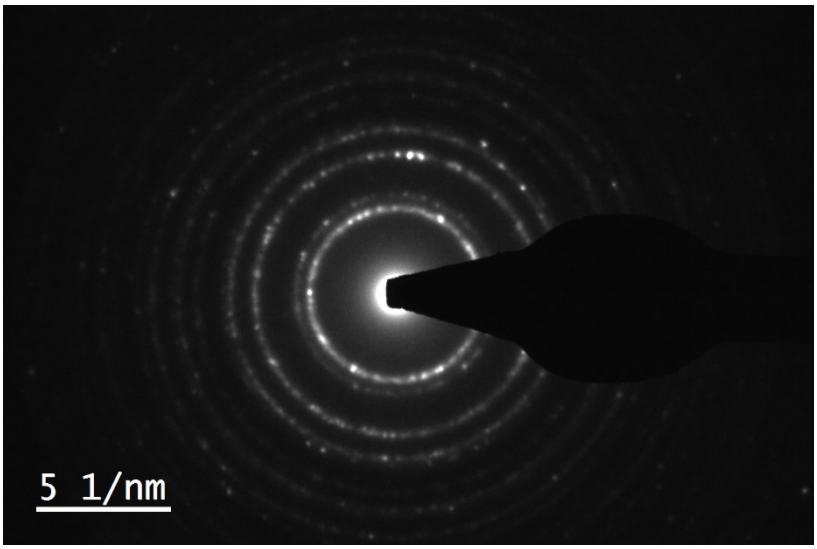

Fig. S2. Electron diffraction of the CeO_2 nanoparticles.

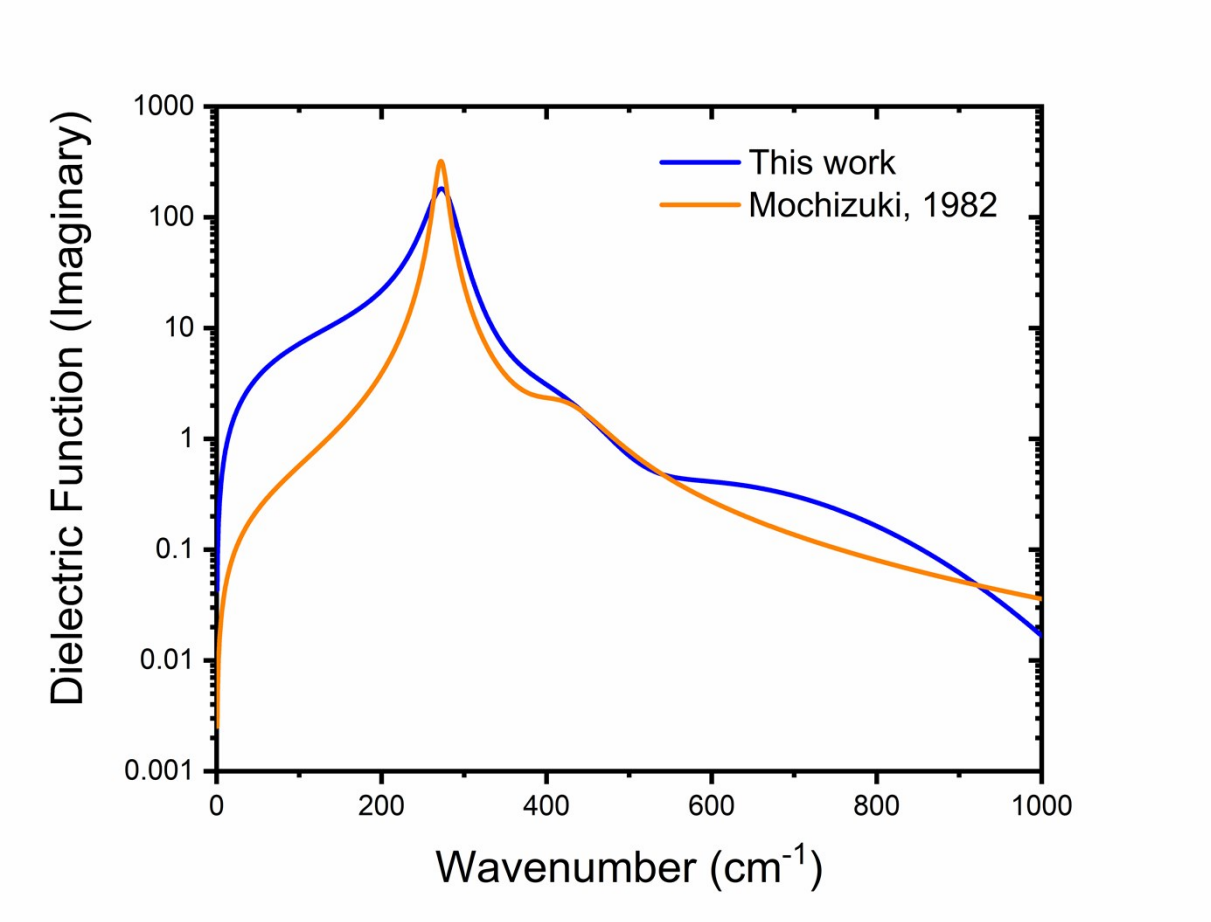

Fig. S3. Logarithmic representation of the imaginary parts of the dielectric functions represented in Fig. 8 of the main text (the nanoceria studied in this work, and a single-crystal model reported in Ref. 32). The secondary features of both functions are more easily appreciated.

z	m_f (z, 0.5 t)	m_f (z, 0.75 t)	m_f (z, 1 t)	m_f (z, 1.5 t)
0.0015	0.8973377	0.99428	1.07755095	1.24285
0.0025	4.91762142	5.448888	5.90523237	6.81111
0.004	3.41142834	3.779976	4.09654899	4.72497
0.008	1.14113544	1.264416	1.37031084	1.58052
0.014	0.695036188	0.7701232	0.834621018	0.962654
0.021	1.01612836	1.125904	1.22019846	1.40738
0.036	0.7564033	0.83812	0.90831255	1.04765
0.047	0.721175476	0.7990864	0.866009886	0.998858
0.066	0.57388892	0.635888	0.68914362	0.79486
0.085	0.524544552	0.5812128	0.629889372	0.736516
0.109	0.472445032	0.5234848	0.567326652	0.684356
0.142	0.465961472	0.5163008	0.559540992	0.645376
0.183	0.40846789	0.452596	0.490500915	0.565745
0.22	0.371722422	0.4118808	0.446375817	0.514851
0.272	0.304639958	0.3375512	0.365821113	0.421939
0.343	0.238683092	0.2644688	0.286618062	0.330586
0.437	0.187862234	0.2081576	0.225590799	0.260197
0.551	0.158310052	0.1754128	0.190103622	0.202661
0.667	0.07577029	0.083956	0.090987315	0.104945
0.797	0.07577029	0.083956	0.090987315	0.0494515
0.923	0.0408584132	0.04527248	0.0490640502	0.0265906
1	0	0	0	0

Table S1. Anchor points for the Bergman spectral density.

Parameter	Value	Units
ε_∞	6.200	-
$\Delta\varepsilon$	23.28	-
Ω_0	273.2	cm^{-1}
Main Gaussian #1		
Area	17.43	-
Mean	428.9	cm^{-1}
Width	132.1	cm^{-1}
Main Gaussian #2		
Area	24.36	-
Mean	142.3	cm^{-1}
Width	341.8	cm^{-1}
Suppl. Gaussian #1		
Area	0.414	-
Mean	566.3	cm^{-1}
Width	402.9	cm^{-1}
Suppl. Gaussian #2		
Area	0.375	-
Mean	1338	cm^{-1}
Width	143.1	cm^{-1}
Suppl. Gaussian #3		
Area	0.598	-
Mean	1578	cm^{-1}
Width	153.2	cm^{-1}

Table S2. Parameters required for retrieving the dielectric function used in the paper (Eq. 6). Main Gaussians are to be found in the denominator of the anharmonic phonon expression, while supplementary ones are added as independent absorption bands. Mathematical expressions for these causal Gaussian functions are found in [1].

[1] D. de Sousa Meneses, J.-F. Brun, P. Echegut and P. Simon, *Applied Spectroscopy*, 2004, 58, 969–974.