

# Supporting information: Insights about the surface of colloidal nanoclusters from their vibrational and thermodynamic properties

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In this document, we give the supplementary information concerning the weighted average frequency of optical modes with surface character, the cluster sizes vs. number of atoms, and the description of the videos showing the surface vibrational modes.

## I. WEIGHTED AVERAGE FREQUENCY OF OPTICAL MODES WITH SURFACE CHARACTER

The weighted average frequency of optical modes with surface character is defined as  $\bar{\omega} = \frac{\int \omega D(\omega) d\omega}{\int D(\omega) d\omega}$  and the values are given in Table. I.

## II. CLUSTER SIZES VS NUMBER OF ATOMS

The cluster sizes versus number of atoms for the nanoclusters we studied are given in Table. II.

## III. VIDEOS

In this part, we present the movies of the passivant rotation mode, shear mode, stretching modes in Video. [1-4], respectively. From Video. [1], we see that the passivants rotate around the surface atoms. The shear mode is given in Video. [2]. As shown in this video, the shear modes only exist in case that the surface atoms are terminated by two passivants. Compare to these low frequency passivant modes, the stretching modes with frequencies as high as 1900 and 2270  $\text{cm}^{-1}$  are presented in Video. [3] and [4], respectively. From these videos, we can see that the frequencies of stretching modes are determined by the bond strength of different types of atom.

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TABLE I: Weighted average frequency of optical modes with surface character

NCs	$\bar{\omega}$ ( $\text{cm}^{-1}$ )	NCs	$\bar{\omega}$ ( $\text{cm}^{-1}$ )
$\text{In}_{321}\text{P}_{312}\text{H}_{300}^*$	336.9	$\text{Cd}_{321}\text{Se}_{312}\text{H}_{300}^*$	189.6
$\text{In}_{321}\text{P}_{312}\text{C}_{300}^*$	356.2	$\text{Cd}_{321}\text{Se}_{312}\text{C}_{300}^*$	195.3
$\text{In}_{321}\text{P}_{312}\text{O}_{300}^*$	355.5	$\text{Cd}_{321}\text{Se}_{348}\text{O}_{300}^*$	195.3
$\text{In}_{321}\text{P}_{312}\text{O}_{300}^*$	353.7	$\text{Cd}_{321}\text{Se}_{312}\text{P}_{300}^*$	195.3

TABLE II: Cluster sizes vs. atom numbers

NC	radius ( $\text{\AA}$ )	NC	radius ( $\text{\AA}$ )
$\text{In}_{225}\text{P}_{240}\text{H}_{228}^*$	13.6	$\text{Cd}_{225}\text{Se}_{240}\text{H}_{228}^*$	14.6
$\text{In}_{321}\text{P}_{312}\text{H}_{300}^*$	14.5	$\text{Cd}_{321}\text{Se}_{312}\text{H}_{300}^*$	15.5
$\text{In}_{369}\text{P}_{348}\text{H}_{300}^*$	15.6	$\text{Cd}_{369}\text{Se}_{348}\text{H}_{300}^*$	17.2

TABLE III: Videos of vibration

Video	File name	Mode	Cluster	Frequency( $\text{cm}^{-1}$ )
[1]	rotation.mp4	passivant rotation mode	$\text{In}_{321}\text{P}_{312}\text{H}_{300}^*$	446.5
[2]	shear.mp4	passivant shear mode	$\text{In}_{321}\text{P}_{312}\text{H}_{300}^*$	777.4
[3]	stretching_low.mp4	passivant stretching mode	$\text{In}_{321}\text{P}_{312}\text{H}_{300}^*$	1898.5
[4]	stretching_high.mp4	passivant stretching mode	$\text{In}_{321}\text{P}_{312}\text{H}_{300}^*$	2268.3