NANO LETTERS

2007
Vol. 7, No. 3
853

Additions and Corrections

Vol. 6, 2006

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Chain-Length-Dependent Vibrational Resonances in Alkanethiol Self-Assembled Monolayers Observed on Plasmonic Nanoparticle Substrates.

Page 2619. Figures 3A and 4A mistakenly presented spectra calculated from the initial guesses for the 1D model parameters, rather than the scaled parameters (see Supporting Information) used in the rest of the paper in the version published on the Web on October 20, 2006 (ASAP) and published in the November 2006 issue (Vol. 6, No. 11, pp 2617−2621). Corrected figures are presented below. The experimental methanethiol Au-S frequency should read 279 (not 270) cm^{-1}. The caption of Figure 2 should read $(CH_2)_{n-2}$, not $(CH_2)_n$.

The DFT functional should be referred to as "PBE1PBE" instead of "PBE".

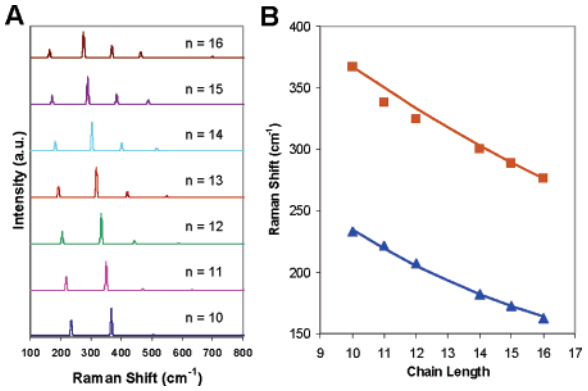

Figure 3. (A) One-dimensional model results for SERS spectra of (Au surface)-S-$(CH_2)_n$-H, for $n = 10$ (decanethiol, bottom) to $n = 16$ (hexadecanethiol, top). Simulated spectra are plotted with a uniform Gaussian broadening of 10 cm^{-1}. (B) Frequencies of the two narrow, intense peaks in the Au-S-$(CH_2)_n$-H spectra of Figure 1B, plotted as a function of chain length (where for the LAM-k peak frequencies, blue triangles are $k = 1$ and orange squares are $k = 2$ from experiment, and blue line is $k = 1$ and orange line is $k = 2$ obtained from the 1D model in (A).

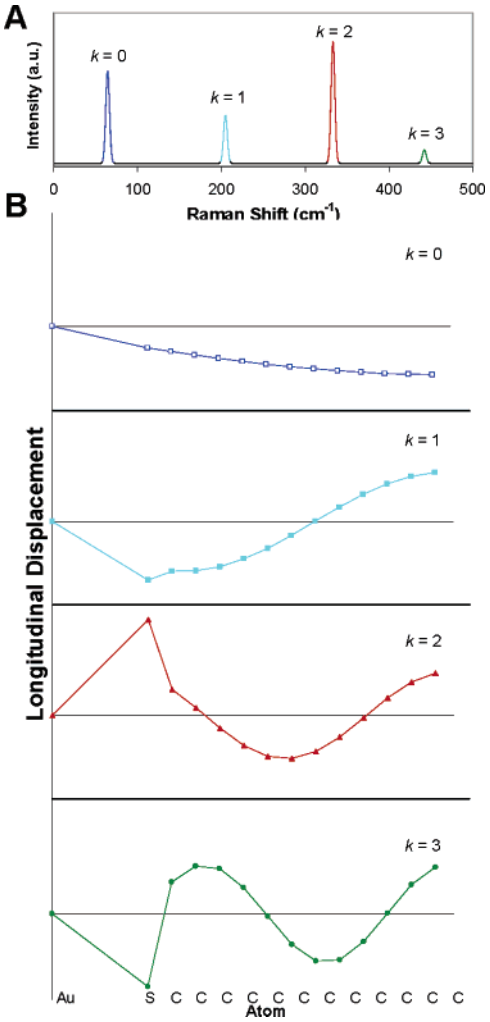

Figure 4. (A) SERS spectra of (Au surface)-S-$(CH_2)_{12}$-H, as predicted by the 1D model. The x-axis begins at 0 cm^{-1} in order to include the $k = 0$ mode. (B) Normal mode eigenvectors for the four vibrational modes shown in (A). The longitudinal displacement of each atom is plotted on the y-axis. The $k = 0$, $k = 1$, $k = 2$, and $k = 3$ modes occur at 64, 205, 333, and 442 cm^{-1}, respectively. The Au−S bond stretch is maximized for the modes with $k = 2$ and $k = 3$ internal nodes (blue open squares are $k = 0$, cyan squares are $k = 1$, red triangles are $k = 2$, green circles are $k = 3$).

NL070254J

10.1021/nl070254j
Published on Web 02/22/2007