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Complementary enhanced solar thermal conversion performance of core-shell nanoparticles

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HIGHLIGHTS

- Optical properties of core-shell NPs were discussed systematically.
- Absorption efficiency can be adjusted by the core-shell or mixing ratios of NPs.
- Optimized parameters of the core-shell NPs for solar absorption were obtained.
- Efficiency of Au-decorated SiO_2 NPs was superior to Au NPs and SiO_2 NPs.

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ABSTRACT

In this study, the properties of various types of core-shell nanoparticles (NPs) were evaluated using the finite difference time domain (FDTD) method towards the enhancement of solar absorption performance. Results showed that the resonance wavelength of SiO_2@Au NPs lay in the 540–900 nm range, covering the near-infrared and visible regions. The resonance wavelength of SiO_2@Ag NPs lay in the 390–830 nm range, covering the entire visible region. SiO_2@Au nanofluid with a core-shell ratio of $\varphi = 0.2$ exhibited the highest solar absorption efficiency with 64% less Au consumption compared to pure Au NPs. For mixed nanofluids, the mixtures featuring core-shell ratios of 0.1 and 0.6 with mixing ratios of 0.5 for SiO_2@Au and 0.6 for SiO_2@Ag gave the highest absorption efficiencies. In addition, the peak solar absorption efficiency of a mixed nanofluid of SiO_2@Au ($\varphi = 0.1$) and SiO_2@Ag ($\varphi = 0.4$) with a mixing ratio of 0.58 was as high as 94.4%. Solar thermal conversion experiments revealed that, under the same conditions, a Au-decorated SiO_2 nanofluid showed a comparable efficiency to the calculated solar absorption efficiency of the SiO_2@Au core-shell nanofluid (~95.2%); it was as high as 95.9%, higher than those of Au NPs and SiO_2 NPs. These results showed that adjusting the core-shell ratios and tuning the mixing ratios of different nanofluids are two efficient methods to enhance the solar absorption efficiencies of SiO_2@Au and SiO_2@Ag NPs under the optimal conditions.

1. Introduction

The energy crisis is one of the key issues in the modern world that must be overcome, and because of it, there are urgent demands for developing clean and sustainable energy sources for our future development [1,2]. Solar energy is a widespread and clean energy source. Efficient methods to transform solar energy into other forms include photovoltaic conversion [3,4], photochemical conversion [5], and photothermal conversion [6]. One of the most common and convenient methods to utilize solar energy is solar thermal conversion for a thermal storage system [7–10], which has attracted more attention. However, the solar thermal conversion efficiency is still too low at present owing to the application of a single transparent fluid. The development of nanoscale control of nanoparticles (NPs) has enabled researchers to investigate their intense interactions with light for a wide range of applications: photothermal therapy [11], sensing [12], and light harvesting & conversion [13,14]. Moreover, this has shown significant technological interest in the effective harvesting and conversion of solar energy [15].

Recently, the addition of NPs to working media was introduced as a means to enhance either solar absorption or scattering for different conversion methods [16,17]. Nanofluid-based direct absorption solar collectors (DASCs) are a potential alternative to traditional solar collectors owing to the enhanced solar thermal conversion performances

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caused by NPs [18]. For DASCs, one of the key issues is the enhancement of the solar absorption performances of the working fluids to improve collector efficiency at a high working temperature. Therefore, researchers have made great efforts to improve the solar absorption performances of the working fluids. The solar thermal conversion characteristics of Ag NPs under realistic conditions could be enhanced by up to 144% with a very low Ag NP concentration (~6.5 ppm) [19]. An experimental model that accounted for heat loss has been introduced to calculate the solar thermal conversion efficiency of a Au nanofluid (2.5 ppm), which could be up to 200% higher than that of water [20]. These enhanced performances could be attributed to the strong interactions of noble metals Au and Ag between light and NPs, resulting in surface plasmon resonance (SPR) around the NP surface at the resonance wavelength [21,22]. When the oscillation frequency of electrons is equal to the incident light frequency, SPR is significantly strong. Both the absorption and scattering properties of plasmonic NPs are enhanced.

As discussed above, the unique optical, magnetic, and electronic properties of metal NPs enable photothermal, therapeutic, and electronic device applications, respectively. However, the limited range of the properties of simple spherical metal NPs has restricted their ability to function in many of these applications. The use of a shell layer is an efficient way to tune the optical properties of NPs and reduce the consumption of noble metals. Nanoshells, consisting of a dielectric core covered by a noble metal shell layer, also show tunable SPR. The SPR wavelengths are affected by the parameters of the core and shell layers, because of the interaction between the inner and outer surfaces of the metallic shell. For metal semiconductor core-shell nanostructures, the effect of the semiconductor shell on the metal NP, or vice versa, results in reduced charge recombination at the interface, leading to an enhanced efficiency in energy conversion and storage applications such as solar cells, fuel cells, rechargeable batteries, and super capacitors [23]. Tang et al. [24] reported that tuning the aspect ratios of $Au@SiO_2$ core-shell nanorods could lead to increased cross-sectional scattering and spectrally absorbing energy density for perovskite solar cells. Kim et al. [25] reviewed “smart” core-shell composite NPs with multi-response mechanisms, for example, to temperature, light, or an applied magnetic field. Additionally, hydrogel-coated metal@silica NPs have been demonstrated to store drugs in a mesoporous silica interlayer to carry cargo to targeted sites [26]. Core-shell nanostructures have become new potential systems for the enhancement of given properties of the native components; this could be because of the effects of the interface between the core and shell [27]. The key is to develop tailored materials based on core-shell NPs, which would open the way to bifunctional NPs.

The SPR wavelength of nanoshells can be tuned from the visible to the infrared domains [28]; this can be utilized efficiently to tune the radiative properties of plasmonic nanofluids used in solar thermal applications [29]. Results have shown that the structures of composite NPs themselves can simultaneously influence their average and near-field radiative properties and, thus, those of plasmonic nanofluids. In other experiments, the optical absorption of a $TiO_2@Ag$ plasmonic nanofluid within the solar radiation spectrum was enhanced remarkably owing to the SPR effect on the Ag surface [30]. The scattering, absorption, or extinction coefficient for NPs with Si or SiC cores and Au, Ag, Cu, or Al shells were calculated using the Mie scattering theory and the Rayleigh scattering approximation by Wu et al. [31]. Results showed that the coupling effects between light and the core-shell interface can be utilized efficiently to tune the radiative properties of plasmonic nanofluids used in photothermal applications. In addition, the use of carbon@Au core-shell NPs dispersed in liquid water has been proposed for the enhancement of solar thermal energy conversion efficiency; it was demonstrated that carbon@Au NPs can theoretically enhance the intensity of the absorption peak while broadening the absorption band [32]. Li and Wang et al. [33–35] conducted serial experimental studies on the photothermal performance of $Ag@TiO_2$ and other NPs with great absorptivity in the visible region. In the study of Taylor et al. [36], core-shell $Ag@SiO_2$ NPs were dispersed in water to filter out the ideal spectrum for Si photovoltaic cells in hybrid photovoltaic/thermal collectors. These simulation and experimental results from previous studies showed that core-shell NPs could improve solar absorption ability by tuning the absorption peak location or broadening the absorption band. As described above, the improvement of solar absorption efficiency is significantly influenced by the particle material, size, shape, volume fraction, etc. However, simultaneous investigations of the thermal and optical properties have been rare, especially for the spectral properties that are critical for efficiency in photothermal applications. Moreover, optimization of the material design, core-shell ratio, and collector parameters (such as the NP volume fraction and collector height) have not been investigated systematically. New strategies to improve solar absorption performance by matching the NP absorption properties with the solar spectrum intensity are required in addition to these methods.

Hence, in this study, the optical properties of various types of core-shell NPs were evaluated. The optimal combinations of core-shell NPs whose absorption characteristics fit the solar spectrum at the Earth's surface are discussed in this paper; these would result in less noble metal consumption. In addition, the collector height and NP volume fraction were optimized. The solar absorption efficiencies of $SiO_2@Au$ and $SiO_2@Ag$ NPs were enhanced by adjusting their core-shell ratios or tuning their mixing ratios.

2. Theoretical modeling

The extinction coefficient of a nanofluid can be determined by adding the individual contributions of the NPs and base fluid as follows [37]:

$$k_{e\lambda,nf} = k_{e\lambda,np} + k_{e\lambda,bf} \tag{1}$$

where $k_{e\lambda,nf}$, $k_{e\lambda,np}$, and $k_{e\lambda,bf}$ are the spectral extinction coefficients of the nanofluid, NPs, and base fluid, respectively. Therefore, the optical properties of the base fluid (water) and NPs are evaluated separately.

2.1. Optical absorption of the base fluid

Water is used as the base fluid owing to its good absorption in the near-infrared range. In a pure fluid, the effect of scattering can be neglected, so only the absorption effect is considered. Therefore, the spectral extinction coefficient of the base fluid (i.e., water) can be calculated as follows [37]:

$$k_{e\lambda,bf} \approx k_{a\lambda,bf} = \frac{4\pi\kappa}{\lambda} \tag{2}$$

where $k_{a\lambda,bf}$ is the spectral absorption coefficient of the base fluid, κ is the absorption index of water, and λ is the wavelength. Fig. 1 shows the absorption coefficient of water, which indicates that it has poor absorption ability in the ultraviolet and visible light spectral ranges. However, it is a strong absorber in the near-infrared range. Adding NPs to a base fluid can greatly improve the absorption ability in visible light. Therefore, the present study focused on improving solar absorption by changing the NP elements or mixing various NPs to broaden the solar absorption spectra.

2.2. Optical properties of the nanoparticles

In this work, the finite difference time domain (FDTD) method was used to evaluate the optical properties of core-shell NPs, a model of which is shown in Fig. 2(A). An explicit time-marching algorithm is involved in this method for solving Maxwell equations on discretized spatial grids. The electromagnetic propagation in a system can be described by Maxwell equations [38]: