

Quantitative Verification of Microwave Heating Based on IR/FIR Spectrum Analysis

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ABSTRACT

When DFT/MM-derived IR and FIR spectrum of materials is analyzed using their molecular models, their microwave thermal effect will be predicted and verified more quantitatively than the well-known heat output formula, $P = 1/2\sigma|E|^2 + \pi f \epsilon_0 \epsilon_r'' |E|^2 + \pi f \mu_0 \mu_r'' |H|^2$.

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Theoretical physicist Dirac predicted 90 years ago that "many physical chemistry theories could be verified by quantum chemical calculations. In fact, molecular modeling based on density functional theory (DFT/MM) provides IR/FIR (microwave-radio frequency) spectra of the equilibrium three-dimensional molecular structure of substances and materials composed of associated molecules. By converting absorbed energy in the FIR region (500-0 cm^{-1}) to thermal energy in the IR region (2000-500 cm^{-1}), heat generation derived from absorption of microwave and high-frequency energy can be quantitatively verified. We named this heat generation as thermo-upconversion of microwave energy. We have already reported thermo-upconversion for steam [H_2O]₃, water [(H_2O)₃(H_2O)₃], ice [H_2O]₆, transition metal oxides, [Ni_4O_4] and [Fe_2O_3]₂ [1,2].

In order to nobly understand microwave/high-frequency heating, we report that microwave energy is converted into thermal energy by the thermo-upconversion effect for all solid state of silica-based materials, carbon-based materials, and organic polymers.

DFT calculations are performed using the B3LYP exchange correlation functional and the 6-31G(d) basis set with Spartan²⁰ (Wavefunction, Inc. Irvine, CA).

Figure 1 Shows the IR (2000 to 500 cm^{-1})/FIR (500 to 0 cm^{-1}) spectrum of the quartz tube crystal model [$\text{Si}_{15}\text{O}_{22}$]. The thermo-upconversion efficiency of quartz as a representative silica-based material was determined. Since quartz absorbs FIR, i.e., microwave

and radio frequency well and has effective thermo-upconversion, we can evaluate that tubes made of quartz are suitable for use in high-temperature heating under microwave irradiance.

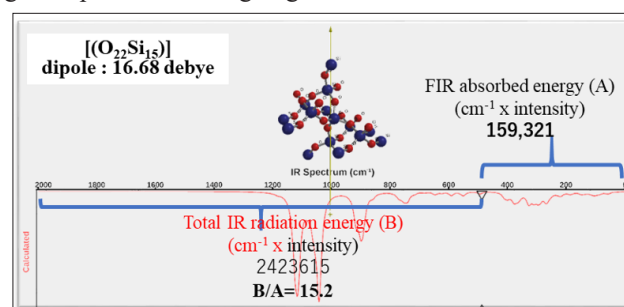


Figure 1: IR(2000-500 cm^{-1})/FIR(500-0 cm^{-1}) spectrum determining the thermal upconversion efficiency of the quartz crystal model [$\text{Si}_{15}\text{O}_{22}$]. The total FIR absorbed energy (A) is obtained by multiplying the wave number giving each lmax by the intensity. The total IR absorbed and radiative (thermal) energy (B) is obtained by multiplying the wave number giving each lmax by the intensity. The value B/A will be a measure of the thermo-upconversion effectiveness. The quartz crystal model [$\text{Si}_{15}\text{O}_{22}$] is from the X-ray single-crystal packing unit structure of quartz, which is obtained from the Cambridge Structural Database.

Figure 2 Shows the IR (2000 to 500 cm^{-1})/FIR (500 to 0 cm^{-1}) spectrum of the model structure of amorphous silica in ceramic [(SiO_2)₃]. It is now verified that amorphous silica absorbs microwaves efficiently, and the heat upconversion index B/A is also effective, which confirms that ceramics containing silica can be efficiently heated under microwave irradiance [3].

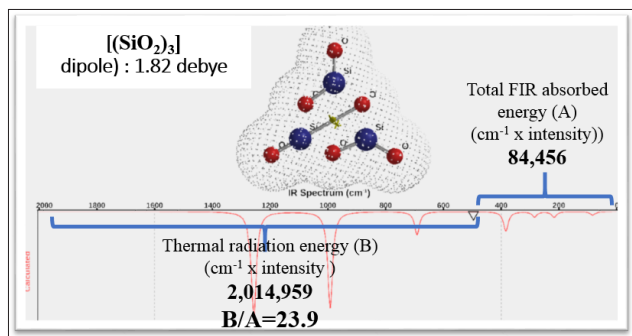


Figure 2: IR(2000-500 cm^{-1})/FIR(500-0 cm^{-1}) spectrum to evaluate thermal upconversion of silica-based ceramic model $[(\text{SiO}_2)_3]$. The total FIR absorbed energy (A), the total IR absorbed energy (B) and the value B/A are shown.

Teflon and polyethylene do not noticeably heat up under microwave irradiance using microwave oven of less than 1 kW output. In order to confirm these facts, the IR/FIR spectra of the Teflon model molecule $[\text{n-C}_{18}\text{F}_{38}]$ and the polyethylene model $[\text{n-C}_{18}\text{H}_{38}]$ are analyzed (Figure 3).

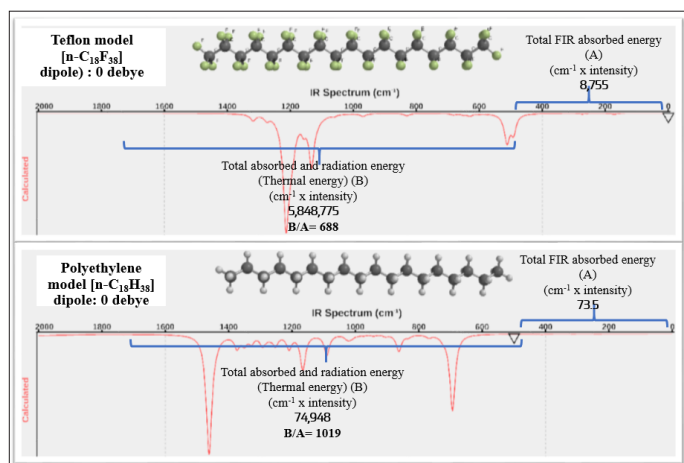


Figure 3: IR(2000 to 500 cm^{-1})/FIR(500 to 0 cm^{-1}) spectra to evaluate the thermal upconversion of Teflon model $[\text{n-C}_{18}\text{F}_{38}]$ and polyethylene model $[\text{n-C}_{18}\text{H}_{38}]$.

It is now verified that both Teflon and polyethylene have a small total energy indicated by A of FIR absorption. However, the B/A value, which is an indicator of the effectiveness of thermo-upconversion, is not small enough. The use of interior materials of Teflon had better not be used when the output of microwave oven is much larger than 1 kW.

Figure 4 shows the IR/FIR spectra of diamond crystal model [d-C₅₂] and the graphene model [g-C₅₂]. It is now verified that both diamond and graphene absorb a large amount of FIR energy indicated by A value. It is also verified that graphene has a significantly high B/A value, proving the graphene will be heated up to high temperature under microwave irradiance.

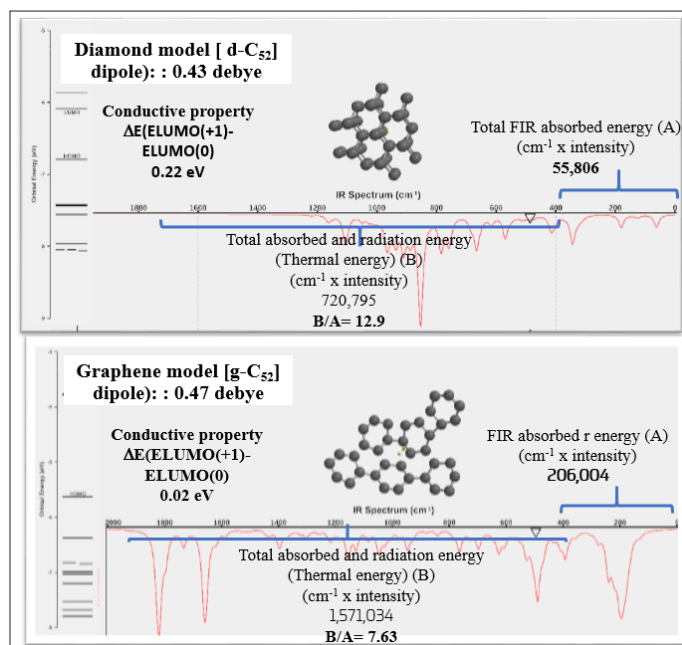


Figure 4: IR(2000 to 500 cm^{-1})/FIR(500 to 0 cm^{-1}) spectra to evaluate the thermal upconversion of Diamond model [d-C₅₂] and Graphene model [g-C₅₂]. The diamond model [d-C₂₂] is from the X-ray single-crystal packing unit structure of diamond, which is obtained from the Cambridge Structural Database.

The heating of graphene to high temperatures under microwave irradiation has been thought to be due to generation of eddy current. In order to verify the generation of eddy current in graphene under microwave irradiation, we determined by molecular modeling that the unoccupied molecular orbital energy levels, E LUMO-0 and E LUMO+1 of the graphene model and compared to that of diamond model. Since electron will travel between molecular orbitals, LUMO+1 and LUMO-0, conducting property can be evaluated from the energy difference between LUMO+1 and LUMO-0 energy level.

The graphene model is determined to have $\Delta E = 0.02$ eV. The ΔE value is significantly smaller than diamond's $\Delta E = 0.22$ eV, and it can also be interpreted that graphene is heated by generating eddy currents under microwave irradiation.

It is known that metals with excellent conductivity do not get heated when irradiated with microwaves. However, it is explained because they reflect the microwave. When we determined the FIR/IR of iron, nickel, and copper models $[\text{Fe}_3]$, $[\text{Ni}_3]$, and $[\text{Cu}_3]$ (Figure 5), these metal models showed absorption peaks only in the far-infrared region. However, it was found that there was no absorption peak in the infrared region. Therefore, it was understood that eddy currents do not occur unless thermal upconversion occurs.

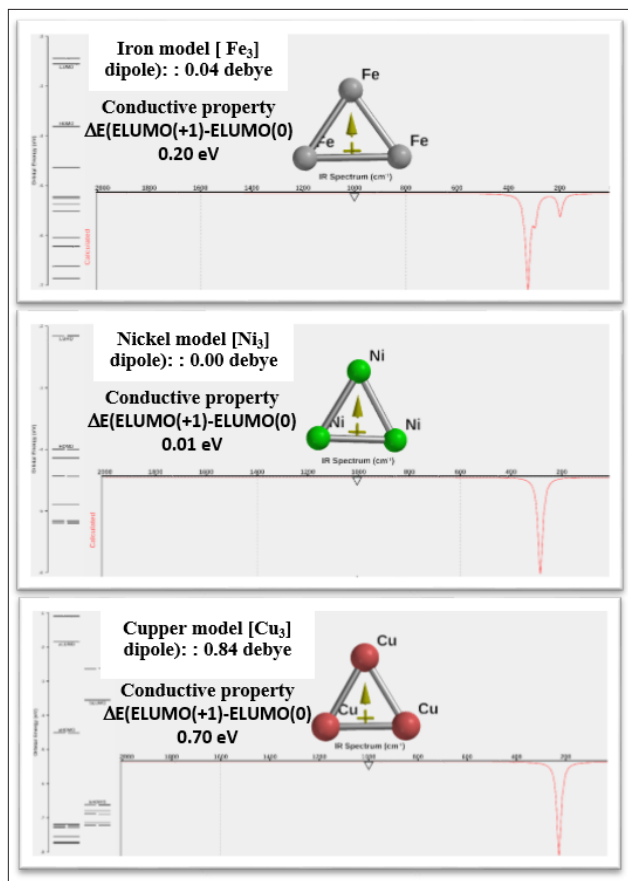


Figure 5: IR/FIR(500 to 0 cm⁻¹) spectra of iron model [Fe₃], Nickel mode [Ni₃], and copper modle [Cu₃] with their conductivity property.

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