

## Radiation Spectral Analysis of 3D Dust Molecular Clusters (PAHs) and Peptoids under Ionization and Electric Field in ISM (Postprint)

**Authors:** Ruiqing Wu, Chunhua Zhu, Guoliang Lü, Xiaojiao Zhang, Xizhen Lu, Jinlong Yu, Wujin Chen and Mengqiu Long

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### Abstract

Polycyclic aromatic hydrocarbons (PAHs), PANHs, and peptoids dust spectral calculations from the interstellar medium (ISM) are important for dust observations and theory. Our goal is to calculate the radiation spectrum of spherical PAHs dust clusters in a vacuum containing ionized and applied in the presence of an electric field. We propose a new simple computational model to calculate the size of three-dimensional spherical dust clusters formed by different initial dust structures. By the Vienna Ab-initio Simulation Package code, the density functional theory with the generalized approximation was used to calculate the electron density gradient and obtain the radiation spectrum of dust. When the radius of spherical dust clusters is  $[0.009-0.042]$  m, the dust radiation spectrum agrees well with the  $Z = 0.02$  mMMP stellar spectra, and the PAHs radiation spectrum of NGC 4676 at wavelengths of  $(0-5]$  m and  $(5-10]$  m, respectively. In the ionized state, the N-PAH,  $C_{10}H_9N$ ,  $2(C_4H_4)_1^+$ , and peptoids  $4(CHON)$ ,  $(C_8H_{10}N_2O_5)_1^+$  dust clusters at  $3.3$  m, while the  $2(C_{22}H_{21}N_3O_2)_1^+$ ,  $4(CHON)$  dust clusters at  $5.2$  m have obvious peaks. There is a characteristic of part of PAHs and peptoids clusters radiation at the near-infrared wavelength of  $2$  m. However, especially after applying an electric field to the dust, the emission spectrum of the dust increases significantly in the radiation wavelength range  $[3-10]$  m. Consequently, the dust clusters of PAHs, PANHs, and peptoids of the radius size  $[0.009-0.042]$  m are likely to exist in the ISM.

## Full Text

### Preamble

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### Radiation Spectral Analysis of 3D Dust Molecular Clusters (PAHs) and Peptoids under Ionization and Electric Field in ISM

Ruiqing Wu<sup>1</sup>, Chunhua Zhu<sup>2</sup>, Guoliang Lü<sup>2</sup>, Xiaojiao Zhang<sup>3</sup>, Xizhen Lu<sup>2</sup>, Jinlong Yu<sup>4</sup>, Wujin Chen<sup>5</sup>, and Mengqiu Long<sup>1</sup>

<sup>1</sup> School of Physics and Electronics, Central South University, Changsha 410083, China; [ruiqingwu163@163.com](mailto:ruiqingwu163@163.com), [mqlong@csu.edu.cn](mailto:mqlong@csu.edu.cn)

<sup>2</sup> School of Physical Science and Technology, Xinjiang University, Urumqi 830046, China

<sup>3</sup> School of Microelectronics and Physics, Hunan University of Technology and Business, Changsha 410205, China

<sup>4</sup> School of Medicine, Xinjiang Medical University, Urumqi 830011, China

<sup>5</sup> School of Medicine, Xinjiang Medical University, Urumqi 830011, China

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### Abstract

Polycyclic aromatic hydrocarbons (PAHs), PANHs, and peptoids dust spectral calculations from the interstellar medium (ISM) are important for both dust observations and theoretical modeling. Our goal is to calculate the radiation spectrum of spherical PAH dust clusters in a vacuum under ionization and in the presence of an applied electric field. We propose a new computational model to determine the size of three-dimensional spherical dust clusters formed from different initial dust structures. Using the Vienna Ab-initio Simulation Package (VASP) code, density functional theory with the generalized gradient approximation was employed to calculate the electron density gradient and obtain the radiation spectrum of dust. When the radius of spherical dust clusters is approximately [0.009–0.042] m, the dust radiation spectrum agrees well with both the  $Z = 0.02$  mMMP stellar spectra and the PAH radiation spectrum of NGC 4676 at wavelengths of (0–5] m and (5–10] m, respectively. In the ionized state, the N-PAH  $C_{10}H_9N$ ,  $2(C_4H_4)^{1+}$ , and peptoids  $4(CHON)$ ,  $(C_8H_{10}N_2O_5)^{1+}$  dust clusters show obvious peaks at 3.3 m, while the  $2(C_{22}H_{21}N_3O_2)^{1+}$  and  $4(CHON)$  dust clusters exhibit peaks at 5.2 m. A characteristic feature of PAH and peptoid cluster radiation appears at the near-infrared wavelength of 2 m. Notably, after applying an electric field to the dust, the emission spectrum increases significantly in the radiation wavelength range [3–10] m. Consequently, dust clusters of PAHs, PANHs, and peptoids with radius sizes of [0.009–0.042] m

are likely to exist in the ISM.

**Key words:** ISM: structure -ISM: molecules -radiation mechanisms: general - (ISM:) dust -extinction

## 1. Introduction

Polycyclic aromatic hydrocarbon (PAH) molecules in the interstellar medium (ISM) contain two or more fused benzene rings and include functional derivatives such as N-PAHs and O-PAHs, primarily composed of the four elements  $^1\text{H}$ ,  $^{12}\text{C}$ ,  $^{14}\text{N}$ , and  $^{16}\text{O}$  [?]. PAHs play a crucial role in the ionization and energy balance of the ISM in galaxies [?, ?], a topic that has attracted widespread interest, particularly since [?] first detected the peptide molecule propionamide ( $\text{C}_2\text{H}_5\text{CONH}_2$ ) in Sagittarius B2(N1).

PAHs constitute an important component of cosmic dust, which originates from stellar winds of asymptotic giant branch (AGB) stars and supernova remnants (SNRs), as well as from nova ejecta in astrophysical theoretical studies. During the post-AGB stellar phase, traces of PAHs can be identified in the stellar spectrum as the stellar temperature increases, because PAHs require energy from ultraviolet (UV) or optical radiation to support their radiative energy and form infrared spectra [?, ?, ?, ?, ?, ?, ?, ?, ?].

PAHs are frequently observed in various astrophysical environments, including the Milky Way (MW), Seyfert galaxies, and starburst galaxies [?, ?, ?, ?]. They exhibit prominent emission characteristics at wavelengths of 3.3, 5.25, 5.7, 6.0, 6.2, 6.7, 7.4, 8.3, 8.6, 10.5, 11.0, 12.0, 13.6, 14.2, 15.8, 16.4, 17.4, and 17.8  $\mu\text{m}$  [?, ?, ?, ?, ?, ?]. Interstellar dust affects galaxy appearance by attenuating short-wavelength radiation from stars and ionized gas while emitting in infrared (IR), far-infrared (FIR), and even near-infrared (NIR) bands. In observed infrared spectra, some Unidentified Infrared Emission (UIE) features appear in nebular spectra, such as at 3.3  $\mu\text{m}$  and 2  $\mu\text{m}$  in the reflection nebula NGC 2023, which have lacked definite physical separation and chemical carrier identification for decades [?, ?, ?].

[?] and [?] suggested that onion-like (3D spherical) nanostructures in the ISM likely grow through layer-by-layer adsorption and evolution. While we do not calculate the chemical reactions and growth processes of dust structures here, our calculations based on initial unit radiation spectra show that the precise size of dust ranges from (4.5  $\text{\AA}$ -0.4)  $\mu\text{m}$  [?, ?]. In diffuse ISM, massive amounts of dust are exposed to a wide range of photon energies, where photoelectric charging could play a significant role in the radiation-stable growth of large dust particles, and complex physical interactions between photons, electrons, and radiation fields may diversify charged PAHs [?, ?]. In photodissociation regions (PDRs) near central stars, numerous escaping photons are produced when dust is irradiated. If the photon absorption rate by dust structures exceeds the collision rate between electrons and surrounding particles, photoelectric charging induces positive charging of particles [?]. Dust is often illuminated by photons

from gamma-ray bursts or active galactic nuclei, and simultaneously prone to Coulomb explosions accompanied by charge heating from high-energy photons [?, ?]. In regions near PDRs, large PAHs are more likely to be ionized and can reach a dicationic state [?, ?]. Dust charge and surface (de)hydrogenation reactions can also affect the optical absorption [?, ?] and radiation spectra of PAHs. The intensity of radiation spectra depends on electromagnetic energy density and emissivity, which are intrinsic material characteristics, as well as inherent temperature and size properties [?].

[?] and [?] investigated the range of photon energies existing in HII regions and the ionization front, studying interactions of PAH cations with UV photons within [9–20] eV. [?] studied electro-optic coefficients as a function of photon energy for  $\text{MoS}_2$ ,  $\text{MoSe}_2$ ,  $\text{WS}_2$ , and  $\text{WSe}_2$ , with photon energies ranging from [0.25 to 4] eV. Electric fields can even cause band-valley splitting and discontinuous structural changes in two-dimensional materials [?]. Dust particles immersed in low-density plasma with direct current or radio frequency discharge acquire large negative charges. When an external electric field breaks the spherical symmetry of the plasma distribution around dust particles, the system of negatively charged dust particles and positive ion clouds becomes polarized and acquires a dipole moment (forming a “dust quasi-atom”). [?] conducted Monte Carlo simulation studies of plasma polarization around dust particles in external electric fields.

In recent years, many research groups have studied dust and heavy element yields ( $^1\text{H}$ ,  $^{12}\text{C}$ ,  $^{13}\text{C}$ ,  $^{14}\text{N}$ ,  $^{15}\text{N}$ , and  $^{16}\text{O}$ ) from AGB stars [?, ?, ?, ?, ?]. Until now, only a few groups have studied PAH dust in the ISM and the relationship between dust size and radiation spectrum. Uncovering the underlying physical relationships among three-dimensional globular clusters, size, ionized dust radiation spectra, and comparative analysis with stellar spectra and PAH radiation characteristics holds significant research importance. The study of PAH content, structure, and shape has deeper implications and impacts. To investigate the effect of photon energy on dust radiation spectra, we consider electric field forces for different field strengths at low photon energies of 4 and 20 eV  $\text{\AA}^{-1}$ . Since PAH dust formation temperatures are as low as 25 K [?], this effect is ignored in this article. The topic of PAH, PANH, and peptoid dust yields is particularly important and fascinating, as it enhances our understanding of PAH origins, fundamental stellar laws, ISM evolution, and dust extinction in observations. Section 2 outlines the physical parameters of our model, detailed results are discussed in Section 3, and conclusions are drawn in Section 4.

## 2. Models and Methods

The physical parameters for the Vienna Ab-initio Simulation Package (VASP) are set as follows: the energy convergence standard is  $1 \times 10^{-6}$  eV, the Hellmann-Feynman force standard is set to  $1 \times 10^{-2}$  eV  $\text{\AA}^{-1}$ , and the vacuum layer is [20–25]  $\text{\AA}$  along the z-direction [?, ?]. The lattice angles of each dust structure are  $\alpha = \beta = \gamma = 90^\circ$ . The vacuum layer prevents dust structures from

interacting with other unit structures. Brillouin zone integration is performed using  $1 \times 1 \times 1$  for static calculations. The calculation employs the Kohn-Sham equation iteration method and projected augmented wave (PAW) pseudopotentials based on density functional theory (DFT) [?]. Structural optimization and corresponding optical spectrum calculations are primarily performed using the Perdew-Burke-Ernzerhof (PBE) functional of the exchange-correlation generalized gradient approximation, with a final plane wave cutoff energy of 400 eV [?, ?, ?].

The optical spectrum of dust can be calculated from the complex dielectric function:

$$\epsilon(\omega) = \epsilon_1(\omega) + i\epsilon_2(\omega)$$

where  $\epsilon_1(\omega)$  and  $\epsilon_2(\omega)$  are the real and imaginary parts of the dielectric function as a function of photon frequency ( $\omega$ ).

The absorption strength  $\alpha(\omega)$  is given by:

$$\alpha(\omega) = (\omega/c) \times \epsilon_2(\omega)$$

where  $c$  is the speed of light. We assume that the reflectivity of smooth dust is approximately equal to its emissivity because the vibrational frequency of electrons around dust atoms does not match the frequency of light waves. When atoms or molecules in excited states transition back to the ground or lower excited state, energy is emitted as new light wave radiation, forming an emission phenomenon [?, ?, ?, ?]. The reflectivity of dust is close to 1.

The emission strength  $E(\omega)$  is calculated by:

$$E(\omega) = (n \times K) / (2\pi)$$

where  $n$  and  $K$  are the real and imaginary parts of the emission index, respectively. The ionization state parameter for dust is implemented by arbitrarily removing [1-2] electrons from the total number of electrons [?, ?, ?, ?]. In the presence of an electric field, the IDIPOL parameter enables monopole/dipole and quadrupole corrections for total energy. In VASP calculations, IDIPOL = 4 obtains the full dipole moment in all directions (see reference 1). Dipoles enable monopole corrections on potentials, allowing potential resets of local potentials and correcting errors introduced by periodic boundary conditions [?].

In the vinylacetylene ( $C_4H_4$ ) molecule model, the optimized lattice constant is calculated as  $a = b = c = 3.277 \text{ \AA}$ , the optimized H-C bond length is (1.07-1.09)  $\text{\AA}$ , and the optimized C-C bond length is (1.47-1.49)  $\text{\AA}$ , consistent with results from [?] and [?].  $C_4H_4$  is a chemical reaction product of  $C_2H_2$ , which has been detected in the spectra of three IR sources embedded in molecular clouds.  $C_4H_4$  is one of five molecules detected after Fourier transform infrared spectroscopy (FTIR) analysis of irradiated acetylene ice [?, ?], making it necessary to study the relevant structural optical properties of this secondary structure.

The cohesive energy of dust is obtained by:

$$E_{\text{coh}} = (n \times E_{\text{H}} + m \times E_{\text{C}} - E_{\text{total}}) / (n + m)$$

where  $E_{\text{H}}$ ,  $E_{\text{C}}$ , and  $E_{\text{total}}$  are the energies of a single  $^1\text{H}$  atom,  $^{12}\text{C}$  atom, and total energy of the monolayer structure  $\text{C}_4\text{H}_4$ , respectively. The physical parameters  $n$  and  $m$  represent the numbers of  $^1\text{H}$  and  $^{12}\text{C}$  atoms in the monolayer structure. The calculated cohesive energy per atom of  $(\text{C}_4\text{H}_4)$  is 5.73 eV, close to the C-H bond energy of 5.7 eV from [?], and comparable to  $\text{Be}_5\text{C}_2$  (4.58 eV per atom) and  $\text{Be}_2\text{C}$  (4.86 eV per atom) [?, ?, ?]. Such high cohesion maintains the structure as a stable connection network, and the molecular structure  $\text{C}_4\text{H}_4$  is considered stable after structural optimization.

We selected the following stable, well-optimized initial structures:  $\text{C}_{36}\text{H}_{16}$  and  $\text{C}_{10}\text{H}_9\text{N}$  (referring to models from [?]), which account for 4.9% and 6.8% of the total PAH content in NGC 4676, respectively, derived from structures in [?] and [?]. The 4(CHNO) is an isomer of isocyanic acid (HNCO) detected in the ISM [?]. The peptoid small molecule 4(CHNO) structure is established according to [?], while the remaining structures  $\text{C}_8\text{H}_{10}\text{N}_2\text{O}_5$ ,  $\text{C}_{22}\text{H}_{21}\text{N}_3\text{O}_2$ , and  $\text{C}_{24}\text{H}_{38}\text{O}_5$  are from models in [?], [?], and [?], respectively.  $\text{C}_8\text{H}_{10}\text{N}_2\text{O}_5$  also contains peptide-like bonds  $1+$  and  $\text{NC}_2\text{O}_1^-$ . The  $\text{C}_{24}\text{H}_{38}\text{O}_5$  PAH structure is compared with peptoid structures containing  $\text{NH}_2$ ,  $\text{H}_2\text{NC}_2\text{O}$ , and  $\text{NH}_4$ .

Astronomical observations from the 1960s found that 3K microwave background radiation exists throughout cosmic space, including vacuum [?]. Gravitational and electromagnetic fields [?] (including radio waves, microwaves, infrared, visible, ultraviolet, and gamma-rays [?]) exist throughout the universe. When an electron meets a positron, they annihilate and convert into a photon—an electromagnetic field. In nuclear fields where photon energy is sufficiently large, photons can convert into electron-positron pairs. Electrons and positrons are physical objects, while photons are electromagnetic fields—that is, vacuum. We consider electrostatic fields applied to different charge magnitudes. The electrostatic field refers to the electric field observed when the observer is at rest relative to the charge. “Static” in electrostatic field has two meanings: absolute static, where both observer and studied charge remain unchanged over time, and relative static, where the studied charge and observer remain relatively stationary. We obviously use a relatively stationary electric field, which regulates photon and electromagnetic field magnitudes. Based on the fact that cationic and electronic actions of nanoparticles dominate main reactions while ignoring other fields, we assume the electrostatic field is equivalent to the harmonic field of the cosmic radiation field at the nanoscale.

[Figure 1: see original paper]

### 3. Results

Our results show that dust clusters with an applied electric field are smaller than those without an electric field, while their radiation spectra remain substantially consistent with stellar spectra. Moreover, 3D dust spectra are consistent with mMMP star spectra and PAHs in NGC 4676 in the band range of (0-10]  $\mu\text{m}$ .

Dust clusters exhibit prominent radiative peaks at wavelengths of 2, 3.3, 5.2, and 6.2  $\mu\text{m}$ , corresponding to observed PAH radiation peaks at 5.2 and 6.2  $\mu\text{m}$ , particularly at [Figure 2: see original paper].

### 3.1. Ionized Spherical Clusters of Dust

Ions interact with surrounding gases, ambient radiation fields (through absorption and photoelectron emission), and other particles (through condensation). These physical processes typically result in dust acquiring non-zero charges, which strongly affect subsequent interactions [?]. On the surfaces of stars associated with photodissociation regions (PDRs), fragmentation dominates for PAH cations, while at photon energies of 13.6 eV in HI regions, ionization channels are expected to be primary [?, ?, ?].

In Figure 1, we plot ideal dust growth as spherical clusters, ignoring intermolecular chemical reactions and bond length changes, and assuming dust clusters form through spherical layer-by-layer growth (referencing [?]). Subgraph (g) shows the central core as the first small dust cluster, with unit area elements taken as our initial molecules  $\text{C}_4\text{H}_4$  or one of six other structures, where the distance from center point O to point P represents the dust cluster radius ( $r_d$ ).

The radiation intensity of spherical clusters ( $F_v$ ) is calculated by:

$$F_v = \Sigma(F_i \times E_i \times \alpha_i \times ds_i)$$

where  $F_i$  is the radiation intensity per unit of initial molecular structure, obtained through Kirchhoff's radiation intensity calculation [?], and  $E$  and  $\alpha$  represent emission and absorption intensities, respectively. The radiant intensity of dust is the flux of radiation produced by central starlight penetrating the dust [?]. Table 1 shows the surface area of unit structures ( $ds$ ) and final radius ( $r_d$ ) of dust clusters for seven initial structures; radiation losses are not considered in this work. The parameter  $r_d$  refers to the final dust size when grown to match the 3D structure and stellar spectrum, while  $r_E$  refers to the final size when the electric field is applied to match the stellar spectrum.

Figures 2 and 3 show that radiation spectra of seven spherical dust cluster types closely match the mMMP stellar radiation spectrum of the Milky Way fitted by [?], indicating such dust structures may exist in the Milky Way. In Figure 2, PAH radiation spectra for neutral structures  $2(\text{C}_4\text{H}_4)$  and  $(\text{C}_{10}\text{H}_9\text{N})$  are more consistent with the fitted stellar spectrum in the near-infrared band [0.5-1.5]  $\mu\text{m}$ . The 1+ or 2+ valence structures show somewhat lower radiation spectra than neutral structures because their absorption spectra are about an order of magnitude higher (see Figure 4).

In Figure 3, peptoid dust shows the opposite result: the radiation spectrum of cationic structures is higher than that of neutral structures. This occurs because the peptoid structure  $(\text{C}_8\text{H}_{10}\text{N}_2\text{O}_5)$  exhibits weaker radiation from ionized structures compared to neutral structures (see Figure 4). The  $4(\text{CHNO})$ ,  $\text{C}_8\text{H}_{10}\text{N}_2\text{O}_5$ , and  $2(\text{C}_{22}\text{H}_{21}\text{N}_3\text{O}_2)$  structures show good consistency with the

mMMP star spectrum in the near-infrared band [0.5-10]  $\mu\text{m}$ . Notably, the  $2(\text{C}_4\text{H}_4)^{1+}$ ,  $(\text{C}_8\text{H}_{10}\text{N}_2\text{O}_5)^{1+}$ , and  $4(\text{CHON})$  structures show a peak at 3.3  $\mu\text{m}$ , while  $4(\text{CHON})$  has a peak at 4.4  $\mu\text{m}$ . The 3.3  $\mu\text{m}$  PAH emissions have also been detected in the NIR spectrum of M82 [?]. [?] noted that IR data from reflection experiments indicated strong radiation peaks at 4.41  $\mu\text{m}$ . [?] observed microwave and millimeter-wave rotational spectra of  $\text{NCO}^{1-}$  in a supersonic beam using Fourier transform microwave spectrometry, with peak values precisely at 3.3  $\mu\text{m}$  [?].

Furthermore,  $2(\text{C}_{22}\text{H}_{21}\text{N}_3\text{O}_2)^{1+}$  and  $4(\text{CHON})$  show a peak at 5.2  $\mu\text{m}$ , close to the minor PAH signature observed by Spitzer/IRS at 5.25  $\mu\text{m}$  [?, ?, ?]. The observed spectrum curve for NGC 4676 was processed by multiplying its original radiation intensity by  $3 \times 10^{-15}$ . Most peptoid structures in the figure pass through the observed spectrum of NGC 4676 from [?], with weak peaks corresponding to wavelengths of 6.2 and 7.4  $\mu\text{m}$ . [?] also show that 65.3 percent of the heteroatomic dust spectrum exists in NGC 4676. Based on the peptoid  $4(\text{CHNO})$  radiation intensity effect, we can well explain why observed PAH dust radiation spectra are higher than theoretical values, as these peptoid heteroatomic radiation spectra may also exist in NGC 4676, although they are often not easily observed. Figure 4 displays absorption and emission spectra for two dust types:  $2(\text{C}_4\text{H}_4)$  and  $\text{C}_8\text{H}_{10}\text{N}_2\text{O}_5$ . Finally, we observe that PAH dust radiation spectra in the ionized state have prominent peaks at near-infrared wavelengths of 0.6, 0.65, 0.8, 1.0, 1.5, 1.8, 2.0, and 2.5  $\mu\text{m}$ , while many near-infrared PAH and peptoid radiation eigenvalues remain unverified by current observations.

[Figure 5: see original paper]

### 3.2. Comparison of Spherical Dust Clusters in Ionized State and in the Presence of Electric Field

Inside molecular clouds, dust is shielded from UV radiation but highly penetrated by X-rays/cosmic rays and their secondary products, causing charge changes [?]. Photoionization studies of grain charging provide the basis for galaxy formation models because they involve radiation fields and gas ionization [?, ?, ?]. The radiation field in the interstellar environment also affects dust optical properties, including emission and absorption coefficients. We explore the effect of electric fields on dust radiation spectra by comparing spherical dust clusters in ionized states with those in electric fields.

In Figure 5, radiation spectra for two electric field strengths (4 and 20  $\text{eV } \text{\AA}^{-1}$ ) of  $\text{C}_{36}\text{H}_{16}$  models overlap, both represented by the light blue line. The  $(\text{C}_4\text{H}_4)$ ,  $(\text{C}_{36}\text{H}_{16})$ , and  $(\text{C}_{10}\text{H}_9\text{N})^{2+}$  models show distinct characteristic peaks at 2  $\mu\text{m}$  wavelength. As shown in Table 1, dust cluster radius changes continuously with applied electric field function, with most showing a decreasing trend. When the electric field is applied, spherical cluster radii become smaller while dust radiation spectra remain close to mMMP stellar radiation spectra (see Table 1,

where parameter  $r_E$  is the final radius after electric field application). Only two structures ( $4(\text{CHNO})$ ,  $\text{C}_{24}\text{H}_{38}\text{O}_5$ ) maintain unchanged radii at 0.024 and 0.031  $\mu\text{m}$  for both  $r_d$  and  $r_E$ , while other structures show radius decreases after electric field application.

The emission spectrum of electric field dust is higher than that of ionized dust, particularly obvious in the wavelength range [3–10]  $\mu\text{m}$ , as shown in Figure 7. The  $2(\text{C}_4\text{H}_4)$  model closely matches PAH observed peaks at 6.2 and 8.6  $\mu\text{m}$  when wavelengths are 6.2 and 8.9  $\mu\text{m}$  under electric force fields of 4 and 20  $\text{eV \AA}^{-1}$ . These PAH models with electric fields all have higher radiation spectra than PAH cations and are very close to neutral PAHs. With increasing electric field strength, the radiation spectrum weakens slightly, but the change is not obvious.

In Figure 6, the radiation spectrum changes of PANOH dust clusters after electric field application are consistent with those of PAHs. The  $4(\text{CHNO})$  model radiation spectrum with electric field and the model considering ionization state are in good agreement with the spectrum in the wavelength range (0–10)  $\mu\text{m}$ , suggesting a high probability that numerous clusters composed of peptoid small molecules exist in the local galaxy. The  $(\text{C}_8\text{H}_{10}\text{N}_2\text{O}_5)^{1+}$  model shows a radiation spectrum peak at 3.3  $\mu\text{m}$ , while electric field models ( $\text{C}_8\text{H}_{10}\text{N}_2\text{O}_5$ ) and  $2(\text{C}_{22}\text{H}_{21}\text{N}_3\text{O}_2)^{1+}$  have characteristic peaks at 2  $\mu\text{m}$ . The  $2(\text{C}_{22}\text{H}_{21}\text{N}_3\text{O}_2)$  model has peaks at 0.5 and 0.7  $\mu\text{m}$ , and the  $\text{C}_{24}\text{H}_{38}\text{O}_5$  model has the most peaks in the wavelength range [0.5–1.5]  $\mu\text{m}$  and at wavelengths of 2.2, 2.8, 4.1, and 5.2  $\mu\text{m}$ . These peptoid models have many peaks in ultraviolet and visible wavelengths and show good agreement with stellar spectra. The relationship between electric field magnitude and radiation spectrum is consistent with the third point above for PAHs.

The scale of electroneutral ionized gases is larger than the Debye length, with motions governed primarily by electromagnetic forces exhibiting remarkable collective behavior. Plasma is widespread in the universe, including ionized gas-like materials. [?] studies of plasma dust particle ion trajectories in applied electric fields show that larger dipole moments have a non-monotonic relationship with applied electric field, though for very small electric fields, the dependence on dust particle charge is weak. This explains why dust clusters formed with electric fields are smaller than those without electric fields while considering ionized states, yet provide similar radiation intensity. This demonstrates that the electric field has an inhibitory effect on dust cluster size increase when assuming the same radiation intensity as without electric field application. We calculated to obtain final growth size and determine the maximum dust cluster value. The radius obtained with applied electric field is clearly smaller than without electric field application, leading us to conclude that electric fields suppress radius growth of dust clusters.

Although radiation eigenvalues at 2, 3.3  $\mu\text{m}$  and other wavelengths lack observational verification, we expect breakthroughs from the James Webb Space Telescope (JWST) and the upcoming Chinese Space Station Optical Survey

Telescope (CSST) in the near-infrared spectrometer (NIRSpec) working band of (0.6–5)  $\mu\text{m}$ , hoping this work provides a theoretical basis for dust cluster observations.

#### 4. Conclusions

We calculated radiation spectra of PAH and peptoid dust clusters in ionized states and under applied electric fields, comparing these results with observed mMMP star and NGC 4676 radiation spectra. PAH and peptoid radiation shows characteristic features at near-infrared wavelengths of 2  $\mu\text{m}$  and 3.3  $\mu\text{m}$ . The PAH and peptoid dust cluster structures in ionized states and neutral structures  $2(\text{C}_4\text{H}_4)^{1+}$  and  $(\text{C}_8\text{H}_{10}\text{N}_2\text{O}_5)^{1+}$  show obvious peaks, while  $4(\text{CHON})$  has a peak at 4.4  $\mu\text{m}$ , and  $2(\text{C}_{22}\text{H}_{21}\text{N}_3\text{O}_2)^{1+}$  and  $4(\text{CHON})$  show clear peaks at 5.2  $\mu\text{m}$ . The emission and radiation spectra of dust increase significantly after electric field application, while the absorption spectrum remains unchanged. The  $(\text{C}_8\text{H}_{10}\text{N}_2\text{O}_5)$  model has a peak at 3.3  $\mu\text{m}$  wavelength. The  $\text{C}_{24}\text{H}_{38}\text{O}_5$  model corresponds to optical PAH peaks at wavelengths of 2.2, 2.8, 4.1, and 5.2  $\mu\text{m}$ . Clearly, peptoid clusters are more sensitive to electric fields than dust clusters considering only ionized states. These results suggest that PAH and peptoid structures are basically stable.

[Figure 7: see original paper]

In Figure 7, the spectra of the two selected dust types increase after electric field application, while changes in dust absorption spectra are weaker. These results are very similar to [?] calculations for  $\text{MoSe}_2$  material. Therefore, the radiation spectrum per unit dust structure increases. With increasing electric field strength, the emission spectrum increases more significantly. After electric field application, atoms and electrons gain energy to generate induced polarization, vibrating at certain frequencies to form oscillating electric dipoles that radiate back to the ISM as light waves. We find that dust dipole moments do not change obviously with increasing electric field strength (total electronic dipole moment changes in the range  $[0.001\text{--}0.002] e \cdot \text{\AA}$ ). Total energy changes weaken with increasing electric field strength. Although dipole moments do not change much with electric field, they are closely related to the distance between positive and negative electron pairs, with smaller distances producing smaller dipole moments.

Considering that the main reason for differences between cationic and uncharged particle radiation spectra is the difference in charge number, we randomly subtract one electron from the total molecular electrons to obtain a positively monovalent cation, and similarly subtract two electrons for a positively divalent cation. When molecules containing H, C, and PAHN lose electrons, their absorption coefficient increases, and when emission coefficients change, radiation intensity increases. For peptide molecules containing H, C, N, and O, the opposite occurs. By definition, plasma is an ionized gas-like substance composed of positive and negative ions generated after atoms and atomic groups lose some electrons

through ionization. The macroscopic scale of electroneutral ionized gases is larger than the Debye length, with motions governed primarily by electromagnetic forces exhibiting remarkable collective behavior. Plasma is widespread in the universe, including ionized gas-like materials. [?] studies show that larger dipole moments have a non-monotonic relationship with applied electric field, though for very small electric fields, dependence on dust particle charge is weak.

PAH and peptoid dust clusters are likely to occur near stars in the local galaxy and in NGC 4676 galaxies, while dust with electric field radiation spectra is higher than ionized dust spectra. In ultraviolet and visible bands with wavelengths [0.08–0.7]  $\mu\text{m}$  and infrared band [0.7–10]  $\mu\text{m}$ , the above dust models make outstanding contributions and fit well with mMMP star radiation spectra or observed spectra from NGC 4676. We believe PAH and peptoid dust likely originate from stars in the local galaxy and NGC 4676. The size of dust clusters after electric field application is smaller when fitted to stellar spectra, approximately [1–4.3] times smaller than dust clusters without electric field and considering ionized states.

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