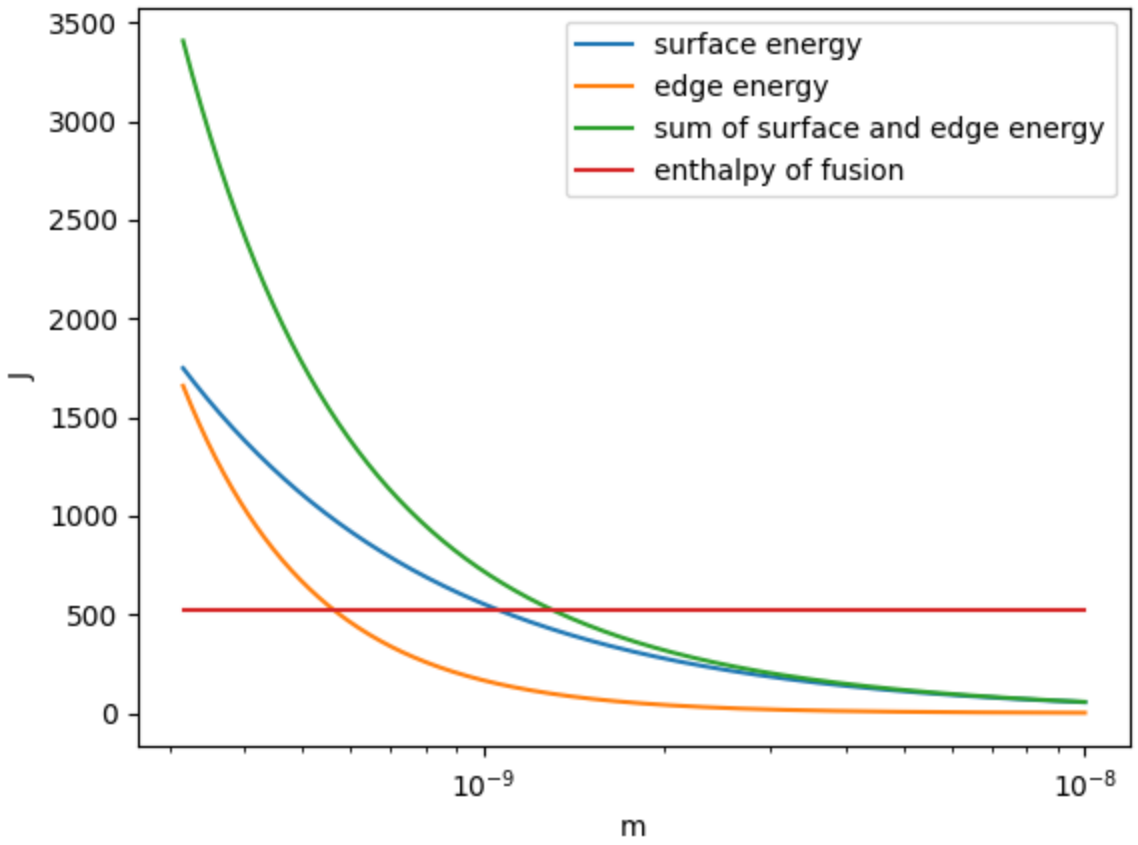
In [2]:
```
%matplotlib widget
import numpy as np
import matplotlib.pyplot as plt
from scipy.constants import pi, Avogadro
```

In [14]:
```
def oppg1ae():
    mass = 1  # 1g NaCl
    density = 2.17  # g / cm^3
    surface_energy_density = 2e-5  # J / cm^2
    edge_energy_density = 3e-13  # J / cm
    enthalpy_of_fusion = 0.52e3  # J / g

    vol = mass / density
    biggest_sidelength = vol ** (1 / 3)
    # sidelength = np.array([biggest_sidelength / (50e4 * n) for n in range(1, 1001)])
    sidelength = np.logspace(-9.5, -8, num=1000) * 1e2

    vol_per_cube = sidelength**3
    num_cubes = vol / vol_per_cube
    total_area = sidelength**2 * 6 * num_cubes
    total_surface_energy = total_area * surface_energy_density

    total_edge_length = sidelength * 12 * num_cubes
    total_edge_energy = total_edge_length * edge_energy_density

    # Conversions to SI units
    sidelength = sidelength * 1e-2
    _, ax = plt.subplots()
    ax.plot(sidelength, total_surface_energy, label="surface energy")
    ax.plot(sidelength, total_edge_energy, label="edge energy")
    ax.plot(
        sidelength,
        total_edge_energy + total_surface_energy,
        label="sum of surface and edge energy",
    )
    ax.plot(
        sidelength,
        np.ones_like(sidelength) * enthalpy_of_fusion,
        label="enthalpy of fusion",
    )
    ax.legend()
    # ax.set_yscale("log")
    ax.set_xscale("log")
    ax.set_ylabel("Energy (J)")
    ax.set_xlabel("Sidelength (m)")
    plt.show()

oppg1ae()
```

Figure



Oppg 1c

About at $a = 1.4nm$

Oppg 1d

Nanoparticles have a lower melting point than bulk NaCl

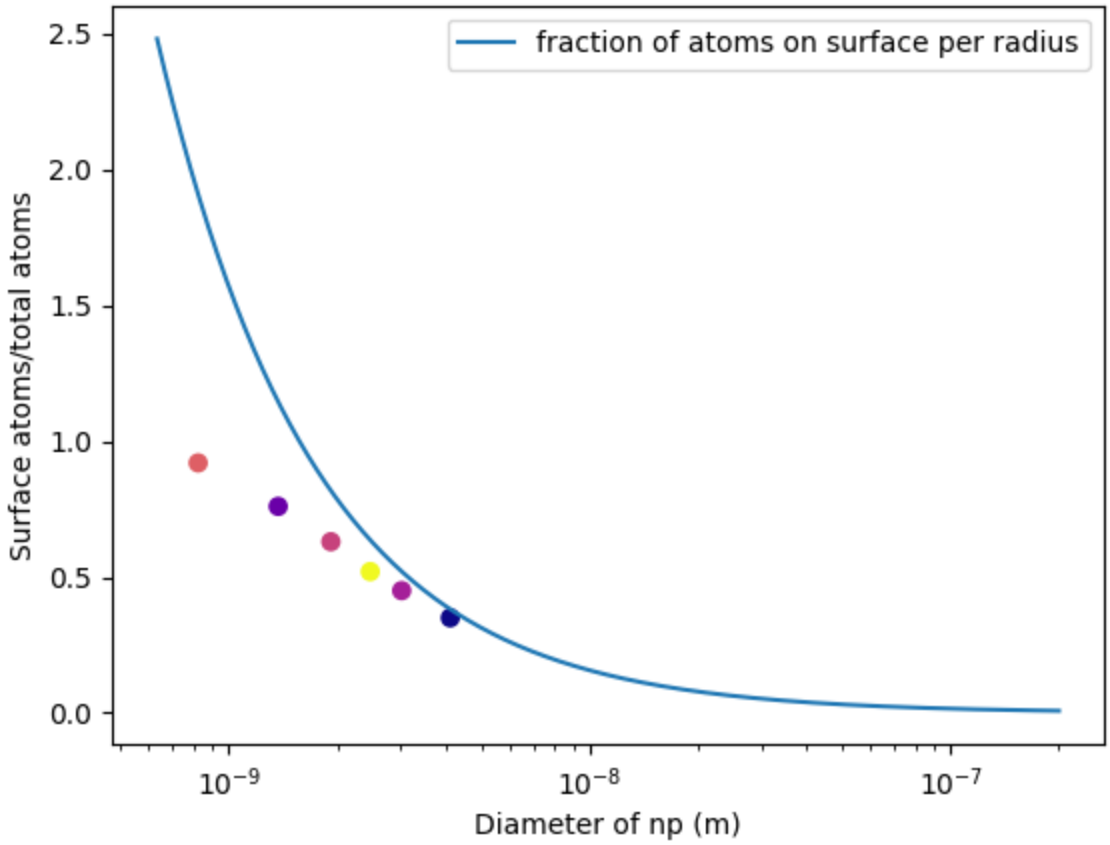
Oppg 1e

We have approximated NaCl to form spheres and that the surface and edge energy to be directly proportional to area and edge length even at low sidelengths. I dont think this will hold experimentally

In [31]:
```python
def oppg1fh():
    mass = 1  # 1g NaCl
    density = 12.0  # g / cm^3
    atomic_radius = 1.37e-8  # cm
    molar_mass = 106.4  # g / mol

    vol = mass / density
    biggest_radius = vol ** (1 / 3) / pi
    smallest_radius = atomic_radius
    # radii = np.linspace(smallest_radius, biggest_radius / 100, 1000)
    radii = np.logspace(-9.5, -7, num=1000) * 1e2
    # radii = np.array([smallest_radius * n for n in range(1, 1001)])
```

```
    volume_of_np = radii**3 * pi

    # Calculate total num
    weight_of_np = volume_of_np * density  # g
    amount_of_atoms = weight_of_np / molar_mass  # mol
    amount_of_atoms = amount_of_atoms * Avogadro  # number

    # one surface atom uses 4 * atomic_radius**2 space on surface
    area_consumed_per_atom = 4 * atomic_radius**2
    surface_of_np = 4 * pi * radii**2
    atoms_on_surface = surface_of_np / area_consumed_per_atom
    # atoms_in_bulk = amount_of_atoms - atoms_on_surface

    fraction_on_surface = atoms_on_surface / amount_of_atoms

    # Make si
    radii *= 1e-2
    diameter = radii * 2
    atomic_radius *=1e-2

    manuals = np.array(
        [
            [(1 * 2 * atomic_radius + atomic_radius) * 2, 0.92],
            [(2 * 2 * atomic_radius + atomic_radius) * 2, 0.76],
            [(3 * 2 * atomic_radius + atomic_radius) * 2, 0.63],
            [(4 * 2 * atomic_radius + atomic_radius) * 2, 0.52],
            [(5 * 2 * atomic_radius + atomic_radius) * 2, 0.45],
            [(7 * 2 * atomic_radius + atomic_radius) * 2, 0.35],
        ]
    )

    _, ax = plt.subplots()
    ax.plot(
        diameter, fraction_on_surface, label="fraction of atoms on surface per radius"
    )
    ax.scatter(manuals[:, 0], manuals[:, 1], c=np.random.rand(6), cmap="plasma")
    ax.legend()
    # ax.set_yscale("log")
    ax.set_xscale("log")
    ax.set_ylabel("Surface atoms/total atoms")
    ax.set_xlabel("Diameter of np (m)")

    plt.show()

oppg1fh()
```

Figure



Oppg 1g

The lower limit of `a` for which the result in `f` makes sense is when `a` is close to the atomic radius

Oppg 2a

The lattice parameter of a metal nanoparticle with a clean surface is affected by nanoparticle size like this: For very small particles, lattice parameter reduces due to dangling bonds. This effect is analogous to the fact that double bonds are shorter than single bonds.

Oppg 2b

For a solid with a *fixed surface area*, the main ways in which the surface energy can be reduced is:

- Binding to similar atoms
- Increase the density of the surface