

VMD Main

File    Molecule    Graphics    Display    Mouse    Extensions    Help

| ID | T | A | D | F | Molecule              | Atoms | Frames | Vol |
|----|---|---|---|---|-----------------------|-------|--------|-----|
| 0  | T | A | D | F | 128w-pos-1_sampled500 | 384   | 1      | 1   |

0 | [Progress Bar] | [Reset]

zoom ☐    Loop     step     speed [Slider]

VMD TkConsole

```
(huangj4) 7 % display resetview
(huangj4) 8 % rotate x by 90
(huangj4) 9 % rotate x by 90
(huangj4) 9 % display resetview
(huangj4) 10 % rotate x by 90
Type 'user add key Escape {my VMD commands...}' to use this key
(huangj4) 11 % display resetview
(huangj4) 12 % rotate x by 90
Type 'user add key Control-2 {my VMD commands...}' to use this key
(huangj4) 13 %
```

x    Main slave    10.15

File Render Controls

Render the current scene using:  
Tachyon (internal, in-memory rendering)

Filename:  
ub/hb\_ihb/0\_prepare/output/Fig1.tga    Browse...

Render Command:  
/usr/bin/open %s    Restore default

Start Rendering

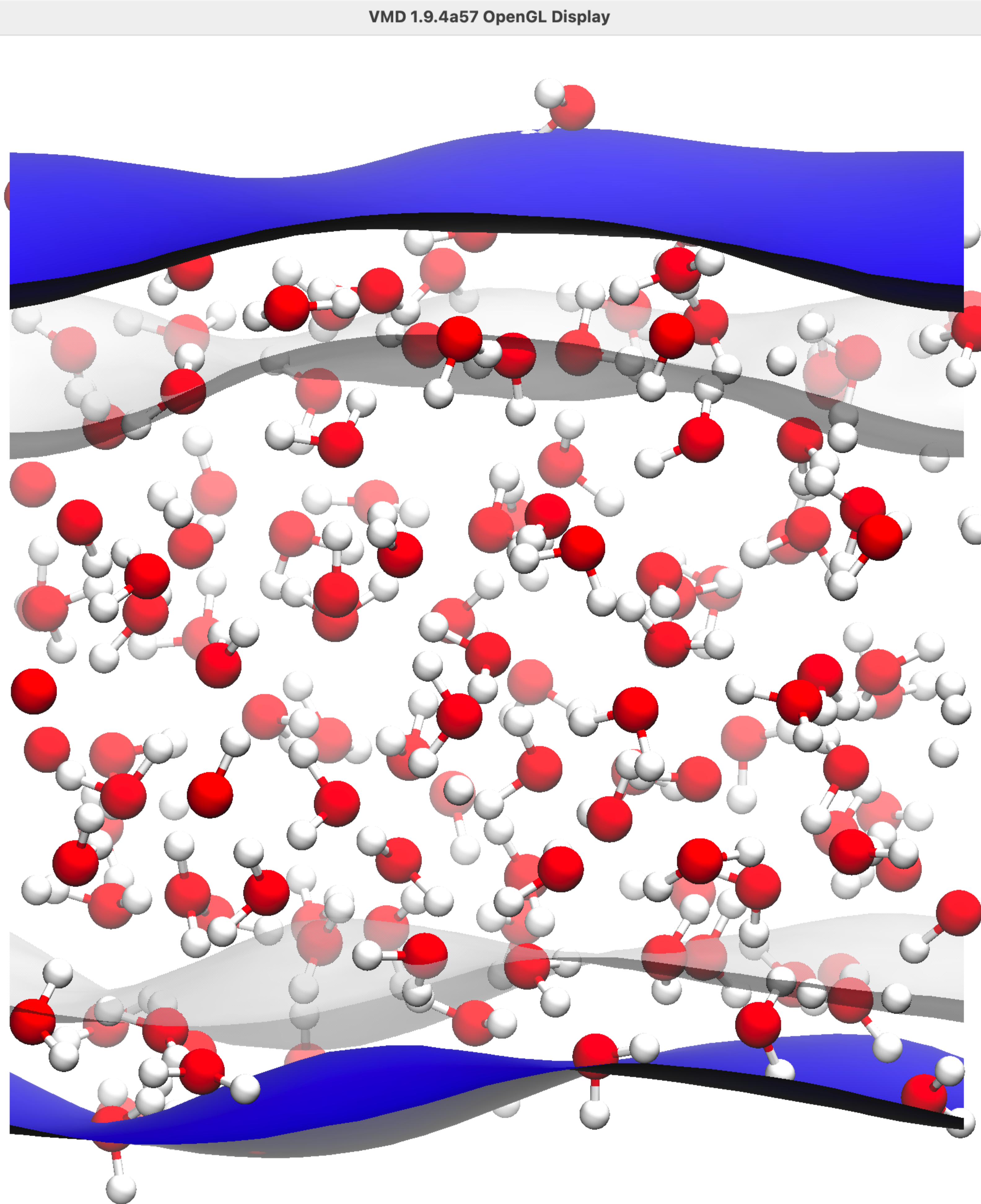
File Render Controls

Render the current scene using:  
POV-Ray 3.6

Filename:  
ub/hb\_ihb/0\_prepare/output/Fig1.pov    Browse...

Render Command:  
-I%s -O%s.tga +D +X +A +FT    Restore default

Start Rendering



Graphical Representations

Selected Molecule  
0: 128w-pos-1\_sampled500.cub

Create Rep    Delete Rep

| Style      | Color    | Selection |
|------------|----------|-----------|
| Isosurface | Molecule | <volume>  |
| CPK        | Name     | all       |
| Isosurface | Name     | <volume>  |

Selected Atoms  
all

Draw style    Selections    Trajectory    Periodic

Coloring Method    Material  
Molecule    Opaque

Drawing Method  
Isosurface    Default

Range 0 39746    Vol vol0: 128w-pos

Isovalue 0.01817

Step 1    Draw Solid Surface

Size 1    Show Isosurface

Apply Changes Automatically    Apply

Graphical Representations

Selected Molecule  
0: 128w-pos-1\_sampled500.cub

Create Rep    Delete Rep

| Style      | Color    | Selection |
|------------|----------|-----------|
| Isosurface | Molecule | <volume>  |
| CPK        | Name     | all       |
| Isosurface | Name     | <volume>  |

Selected Atoms  
all

Draw style    Selections    Trajectory    Periodic

Coloring Method    Material  
Name    AOChalky

Drawing Method  
CPK    Default

Sphere Scale 1.0

Sphere Resolution 500

Bond Radius 0.3

Bond Resolution 500

Apply Changes Automatically    Apply

Graphical Representations

Selected Molecule  
0: 128w-pos-1\_sampled500.cub

Create Rep    Delete Rep

| Style      | Color    | Selection |
|------------|----------|-----------|
| Isosurface | Molecule | <volume>  |
| CPK        | Name     | all       |
| Isosurface | Name     | <volume>  |

Selected Atoms  
all

Draw style    Selections    Trajectory    Periodic

Coloring Method    Material  
Name    Transparent

Drawing Method  
Isosurface    Default

Range 0 39746    Vol vol0: 128w-pos

Isovalue 0.02839

Step 1    Draw Solid Surface

Size 1    Show Isosurface

Apply Changes Automatically    Apply