



Воронежский государственный университет

Использование MPI for Python для организации очереди выполнения при сканировании поверхностей потенциальной энергии

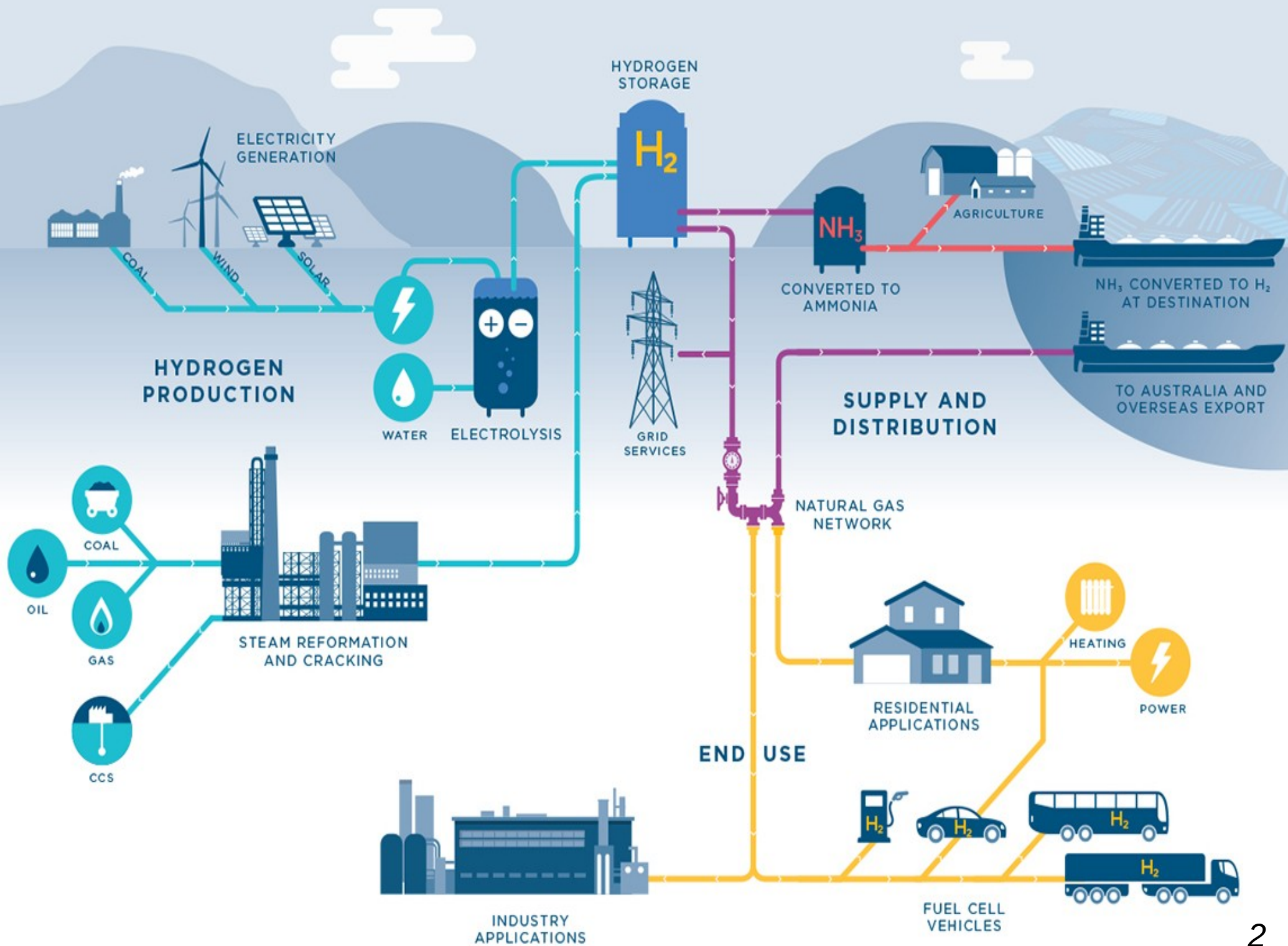
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GENERATION**

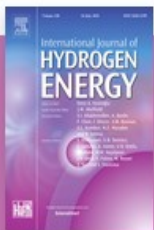
 **Energy
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Александр Романов

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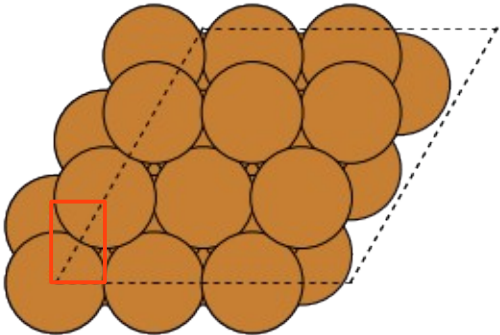
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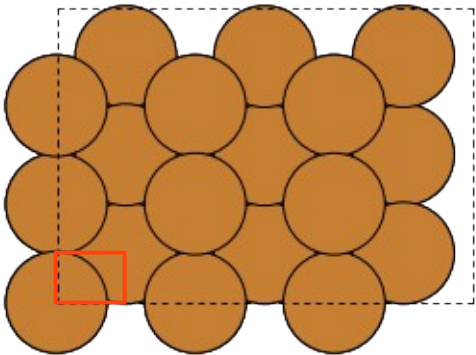
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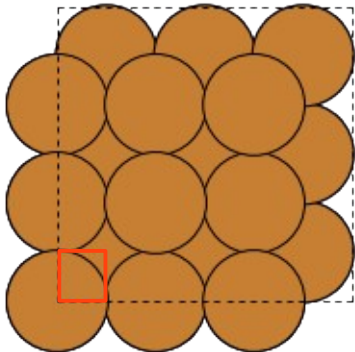
Slab model



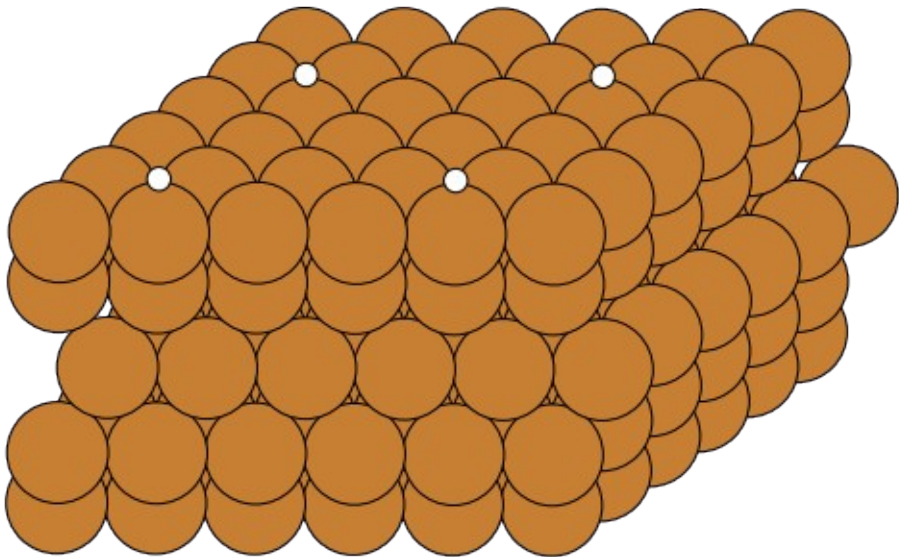
111



110

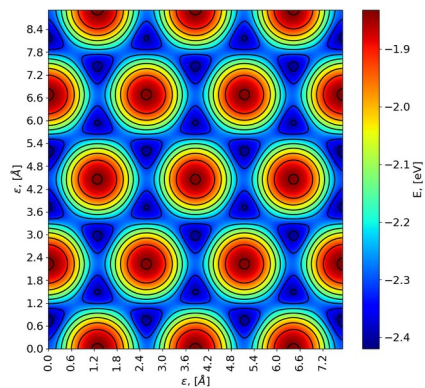
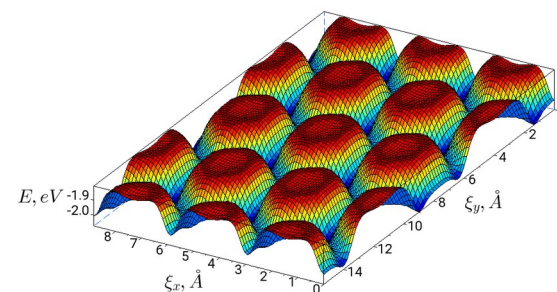
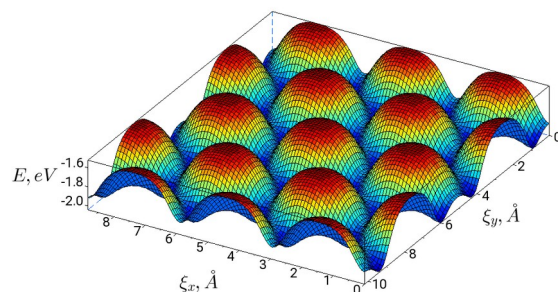
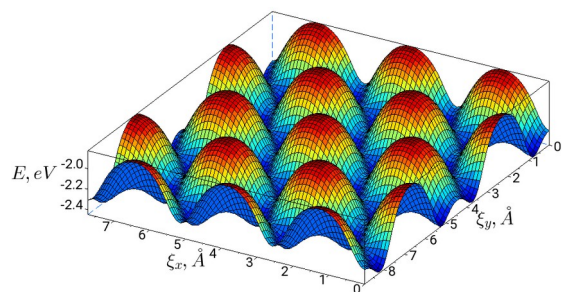
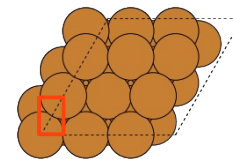


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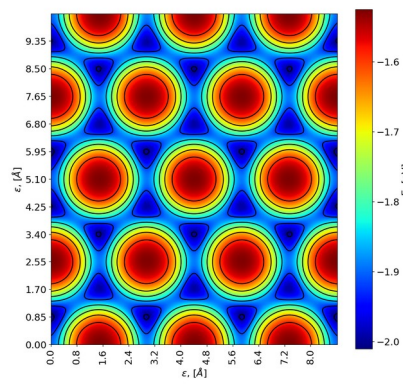




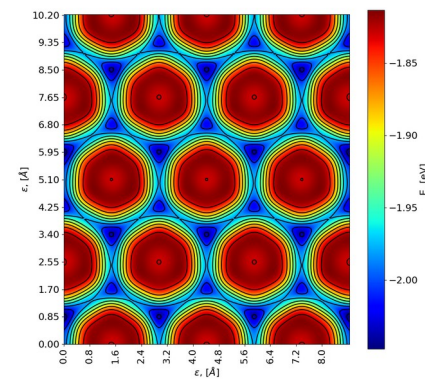
Potential energy surfaces for slabs (111)



Copper



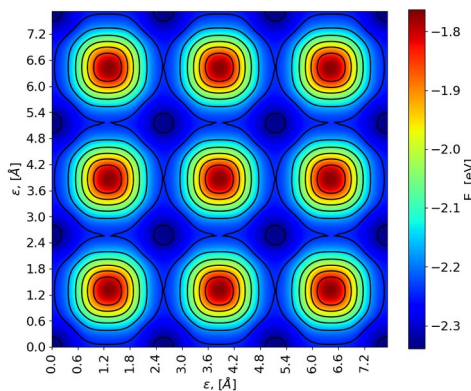
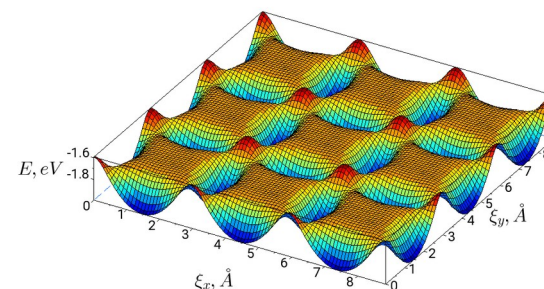
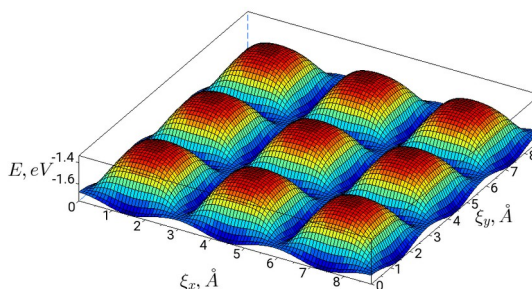
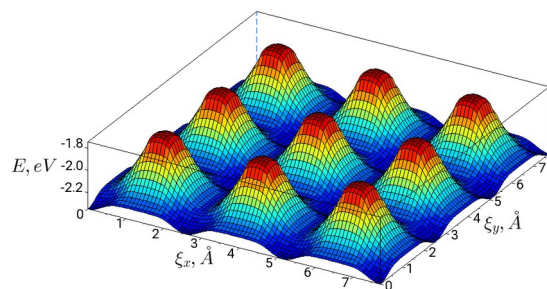
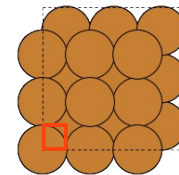
Silver



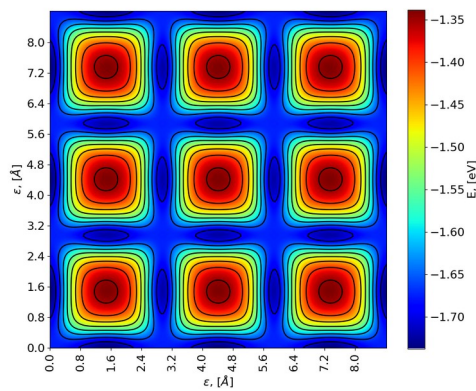
Gold



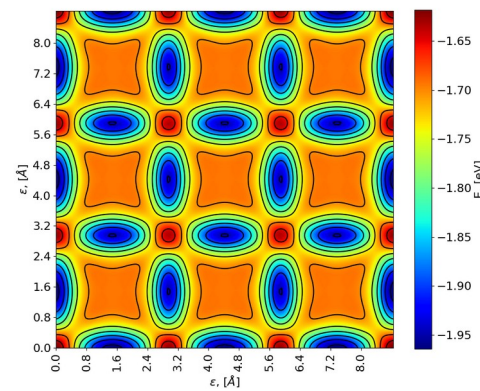
Potential energy surfaces for slabs (100)



Copper



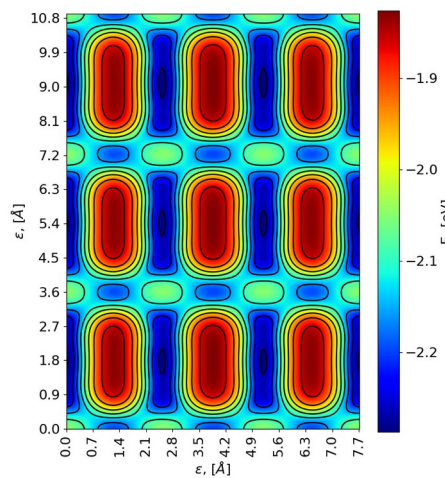
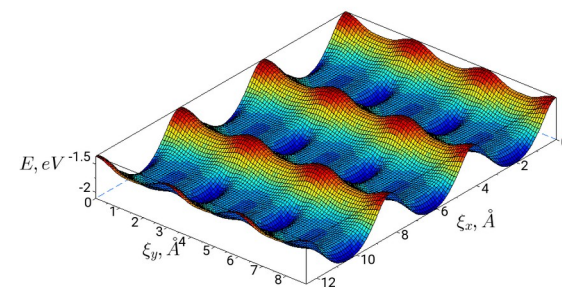
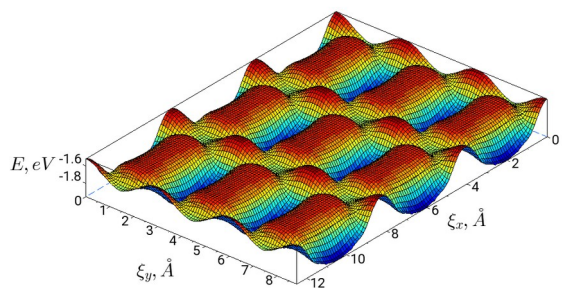
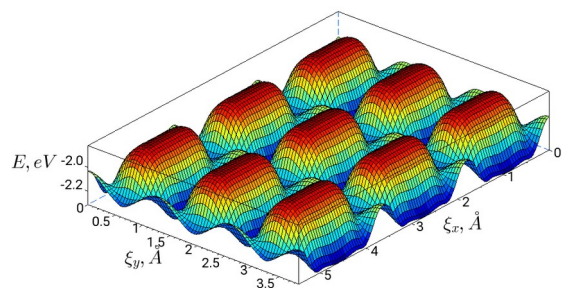
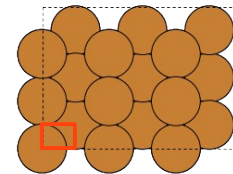
Silver



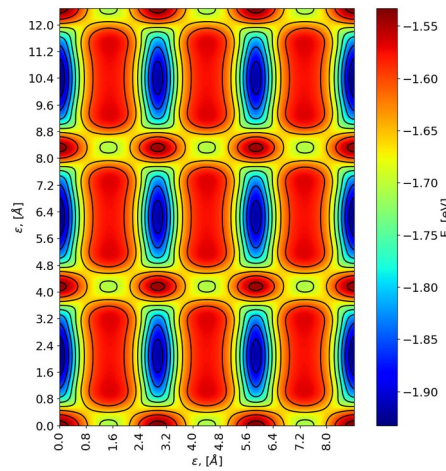
Gold



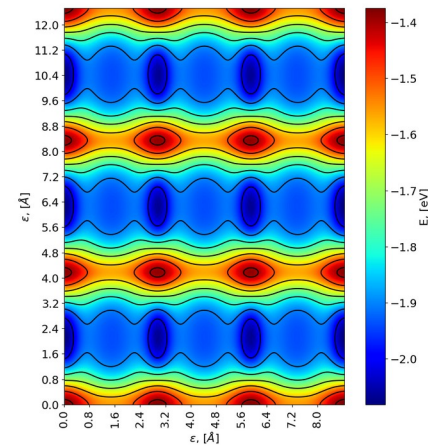
Potential energy surfaces for slabs (110)



Copper



Silver



Gold



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- Workshop focusing on the [extended ASE ecosystem](#) held at CECAM, EPFL, Switzerland June 23-27, 2025

```
from mpi4py import MPI

comm = MPI.COMM_WORLD
rank = comm.Get_rank()

if rank == 0:
    data = {'a': 7, 'b': 3.14}
    comm.send(data, dest=1, tag=11)
elif rank == 1:
    data = comm.recv(source=0, tag=11)
```

```
import queue

q = queue.Queue()

for i in range(5):
    q.put(i)

while not q.empty():
    print(q.get(), end=' ')
```

Thanks for your attention!

