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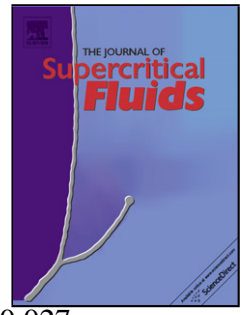

Title: Molecular simulations of supercritical fluid systems

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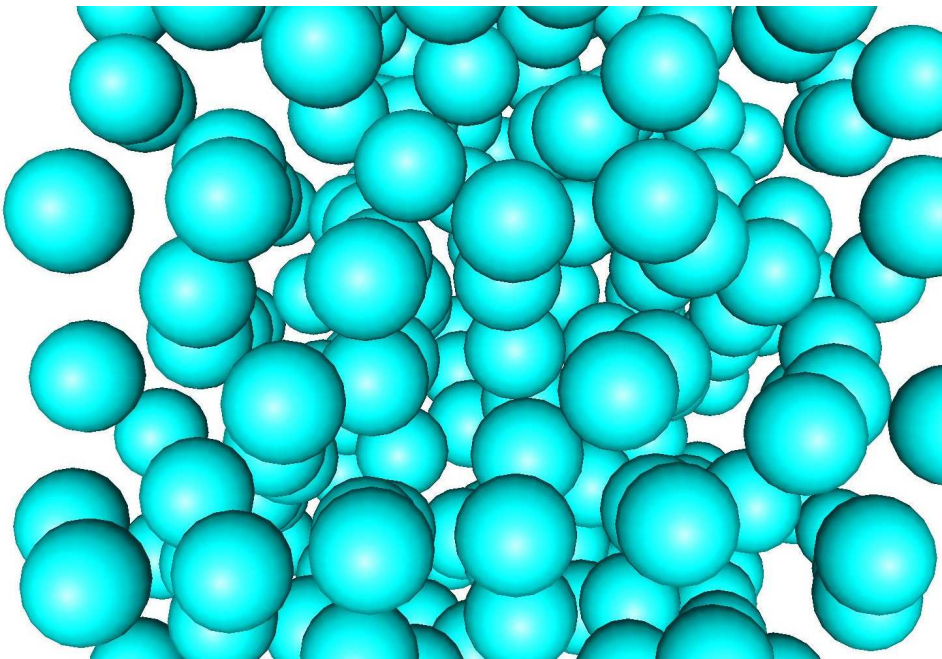
```
energy = 0.0

do i = 1,nmolecules
   do ii = 1,natoms(i)
      do j = i,nmolecules
         do jj = 1,natoms(j)

            lcalculate = .true.

            if (i .eq. j .and. jj .le. ii) then
               lcalculate = .false.
            elseif (i .eq. j .and. lbonded(i,ii,jj)) then
               lcalculate = .false.
            endif

            if (lcalculate) then
               dx = x(i,ii) - x(j,jj)
               dy = y(i,ii) - y(j,jj)
               dz = z(i,ii) - z(j,jj)

               dx = dx - anint(dx/boxlength)*boxlength
               dy = dy - anint(dy/boxlength)*boxlength
               dz = dz - anint(dz/boxlength)*boxlength

               rij = sqrt(dx**2 + dy**2 + dz**2)

               sig = sigma(i,ii,j,jj)
               eps = epsilon(i,ii,j,jj)

               energy = energy + 4.0*eps*((sig/rij)**12-(sig/rij)**6)
            endif

         enddo
      enddo
   enddo
enddo
```



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