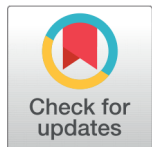# Mechanical properties of YBCO superconductor under high-pressure

B Prabhakar[1]*, **Tanveer Ahmad Wani**[1]

1 Department of Physics, Noida International University, Greater Noida, 201310, India

Abstract

Background/Objectives: The crystal structure of YBCO Superconductor has fascinated the material science research group. The calculation of mechanical properties of YBCO Superconductor under pressure is the main focus in this research work. **Methods/Statistical analysis:** Density Functional Theory calculations using Quantum ESPRESSO under high pressure increasing systematically have been calculated and performed for $YBa_2Cu_3O_7$ Superconductor. The only input required is the lattice parameters at corresponding pressure of materials which are predicted using first principle computational methods at desired high-pressure state. **Findings**: The lattice constants, variations, volume, density, Bulk modulus (B), Young modulus (E), Shear modulus (S) and Poisson ratio (n)values are calculated under pressure up to 30 GPa for YBCO Superconductor. Voigt-Reuss-Hill Approximations, Debye Sound velocities(ϑ_D), Debye temperature(θ_D) and Pugh's ratio(B/G) values have been calculated under pressure for YBCO Superconductor in this research work. **Novelty/Applications:** A larger poisson's ratio value indicates ductile behavior and another criterion often used to differentiate between ductile and brittle behavior is the Poisson's ratio. Poisson's ratio greater than 0.26 implies the ductile behavior. With the application of elastic constants, we have obtained the Debye temperature and other physical quantities of $YBa_2Cu_3O_7$ under pressure.

Keywords: YBCO superconductor; density functional theory (DFT); lattice constants; pressure; quantum ESPRESSO

1 Introduction

The structural phase-transition marked an epoch-making discovery of the phenomenon of superconductivity (SC) (1) by Prof. H. K. Onnes in 1911. Since then, the classical conventional low phase transition-temperature (Tc) superconductivity (CLTSC) (2) was discovered in many systems but the highest Tc~23.2K is resumed in the intermetallic binary A-15 compound Nb3Ge (3). The high-Tc superconductivity (HTSC) is discovered in hole and electron doped cuprates (HTSCC) as [La(R)1-xAx]CuO4±y(LACO) (4), Y(R)A2Cu3O7-y(YACO) (5), Bi2Ca2Sr2Cu3O10(BCACO) (6), Tl2Ca2Sr2Cu3O10 (TCACO) (7) and Hg-doped YACO (HACCO) (8) with Tc~38K, 93K, 110K, 125K, and 164K respectively. The first HTSCC discovered with the Tc ~ 93K (9) for the onset of SC above the boiling point of liquid nitrogen (Tc~77K) is (YBa2Cu3O7-y(YACO), (0.5<y<0.1) with A2+=Ba and having the defect-parvoskite structural state (K2Ni4F6) (9).

The YACO   HTSCC comprises of SC active CuO-AO-CuO2-Y-CuO2-CuO, non-superconducting mediating Y-O, blocking A-O and fluorite [Y(R),A]2O2 layers. The charge carriers are O- holes (L) and hybrid Cu2+ valence states in the quasi two-dimensional (2D) CuO layers of CuO2 square planes and CuO3 chains. The YACO crystallizing in orthorhombic, parvoskite-type structural configuration be such that the O- holes ordering results in an elongation of CuO6 octahedral due to Jahn-Teller (JT) monoclinic structural distortion (10) and there exists coherent finely- twined superstructures along (001) planes of HTSC. The only input required is the lattice parameters at corresponding pressure of materials which are predicted using first principle computational methods at desired high-pressure state and lattice constants are calculated at various pressures. Density Functional Theory (DFT) calculations using Quantum ESPRESSO under pressure increasing systematically have been calculated and performed for YBCO. The calculation values of lattice constants, Bulk modulus (B), Young modulus (E), Shear modulus (S), Poisson ratio (n) versus pressure, Voigt-Reuss-Hill Approximations, Debye Sound velocities(ϑ_D), Debye temperature(θ_D) and Pugh's ratio(B/G) for YBCO Superconductor under pressure investigated in the research method.

2 Theory and computational Details

The examination of strain or stress spreading in the assembly of polycrystalline with respect to two cases. If one is to calculate the average isotropic elastic moduli from the anisotropic single crystal elastic constants, one finds that the Voigt and Reuss assumptions results in the maximum values of theoretical and the minimum calculated values of the elastic moduli respectively. For specific cases orthorhombic lattices, the Reuss shear modulus (G_R) and the Voigt shear modulus (G_V) are

$$G_R = \frac{15}{4(s_{11} + s_{22} + s_{33}) - 4(s_{12} + s_{13} + s_{23}) + 3(s_{44} + s_{55} + s_{66})} \tag{1}$$

$$G_V = \frac{1}{15}(C_{11} + C_{22} + C_{33} - C_{11} - C_{13} - C_{23}) + \frac{1}{5}(C_{44} + C_{55} + C_{66}) \tag{2}$$

The Reuss bulk modulus (B_R) and the Voigt bulk modulus (B_V) are defined as

$$B_R = \frac{1}{(s_{11} + s_{22} + s_{33}) + 2(s_{12} + s_{13} + s_{23})} \tag{3}$$

$$B_V = \frac{1}{9}(C_{11} + C_{22} + C_{33}) + \frac{2}{9}(C_{12} + C_{13} + C_{23}) \tag{4}$$

Hence the elastic moduli of the polycrystalline material can be approximated by Hill's average and for shear moduli it is

$$G = \frac{1}{2}(G_R + G_V) \tag{5}$$

And for Bulk moduli it is

$$B = \frac{1}{2}(B_R + B_V) \tag{6}$$

The Young's modulus E, and Poisson's ratio(n) for an isotropic material are given by

$$E = \frac{9BG}{3B + G} \tag{7}$$

$$n = \frac{3B - 2G}{2(3B + G)} \tag{8}$$

With the above relations, as implemented in thermo pw code, the values have been calculated various modulus of elasticity – Bulk modulus (B), Shear modulus (G), Young's modulus (E) and Poisson's ratio.

The fundamental parameter, Debye temperature(θD) is closely related to the number of atoms, density and wave velocities. From sound velocities the Debye temperature(θD) can be deduced by following equation at low temperature.

$\theta D = h/k_B [\frac{3n}{4\pi}(N_A \rho/M)]^{1/3} V_m$

$V_m = [\frac{1}{3}(2/V_s^3 + 1/V_p^3)]^{-1/3}$

$V_s = \sqrt{G/\rho}$

$V_P = \sqrt{(3 + \frac{4}{3}G)/\rho}$

Where h is planks constant, K_B is Boltzmann constant, n is number of atoms per unit cell, N_A is avagadronumber, ρ is density is molecular weight and V_m, V_S and V_p are the average ,longitudinal and transverse elastic wave velocities.

The calculation of the mechanical properties of YBCO under High Pressure with DFT formalism and Quantum ESPESSO (ver.6.3) have been done in this research paper. The high charge density with method using the PBE-generalized gradient approximation (GGA) for exchange-correlation are presented. The calculated pressure-relevant lattice constants, variations, volume, density, Bulk modulus (B), Young modulus (E), Shear modulus (S), and Poisson ratio (n) etc using a proper pseudo potential and with high suitable value of k-points over IBZ under high cutoff-energy and high charge density with method using the PBE-generalized gradient approximation (GGA) for exchange-correlation are presented .The computations are based on the DFT within the ultra-soft pseudo potential (11) as well as the GGA-PBE (12).

3 Results and Discussion

The constant distance between unit cells in a crystal lattice is known as lattice constant and The lattices constants calculated at different pressures are shown in Figure 1 and the variations versus pressure for YBCO is shown in the Figure 2. The density of a substance is mass per unit volume under certain conditions of temperature and pressure.
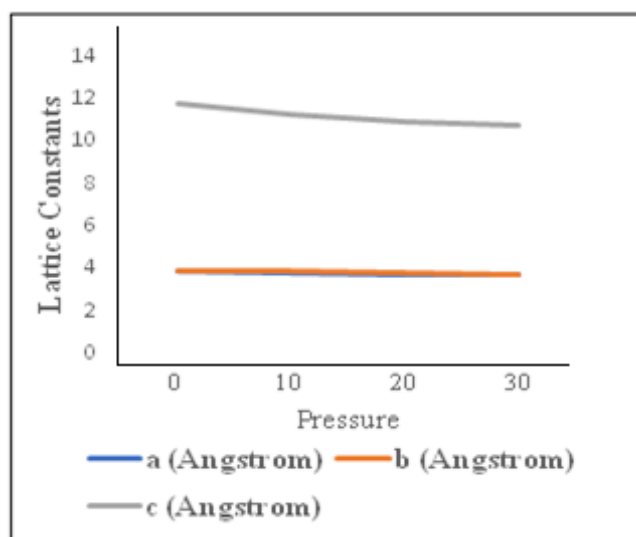

Fig 1. Lattice constants versus pressure for YBCO Superconductor

The variations of volume as well as density are depicted in Figures 3 and 4. All these above calculated values are presented in Table 1. The lattice constants have been calculated as a=3.84467A^O, b=3.92615A^O, c=11.82370A^O at 0 Gpa and a=3.68114A^O,b=3.75638A^O,c=10.71630A^O up to 30Gpa. It can be found that lattice constants are decreases with increasing the pressure, the volume decreases with increasing the pressure and density increasing with pressure.

Table 1. Calculated values of lattice constants, variations, volume and density for YBCO up 30 GPa.

Pressure (GPa)	a (Angstrom)	b (Angstrom)	c (Angstrom)	b/a	c/a	V/V0	Volume (Cubic Angstrom)	Density (g/cm3)
0	3.84467	3.92615	11.82370	1.0212	3.21	2.54	138.7550196	5.7136
10	3.77440	3.85716	11.26770	1.0219	2.99	2.54	139.0150289	6.7993
20	3.72155	3.80267	10.96160	1.0218	2.95	2.40	131.4777606	7.8483
30	3.68114	3.75638	10.71630	1.0204	2.91	2.30	125.7593153	7.4654

With exterior applied pressure or force, distortion arises due to stress and the lattice parameters of the crystal fluctuates with respect to stress with respect to strain. Strain may be defined in another way as the measure of rate of deformation. Bulk modulus
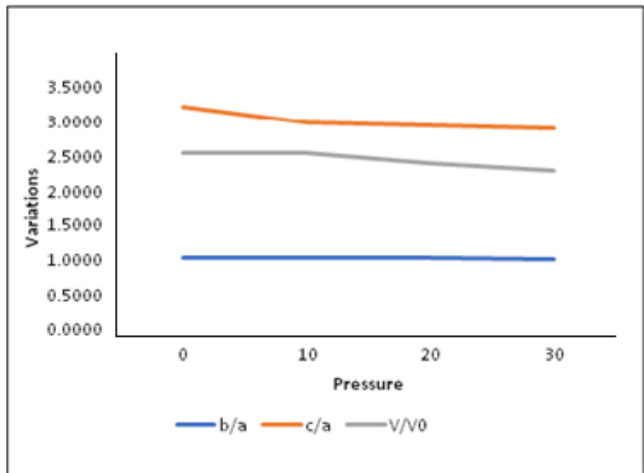
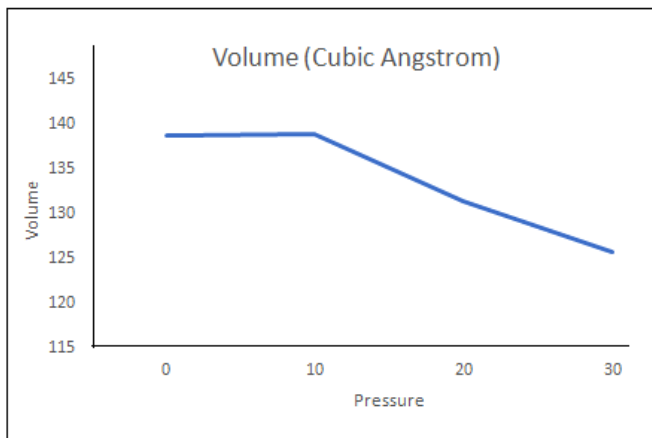**Fig 2.** The variations versus pressure for YBCO Superconductor.

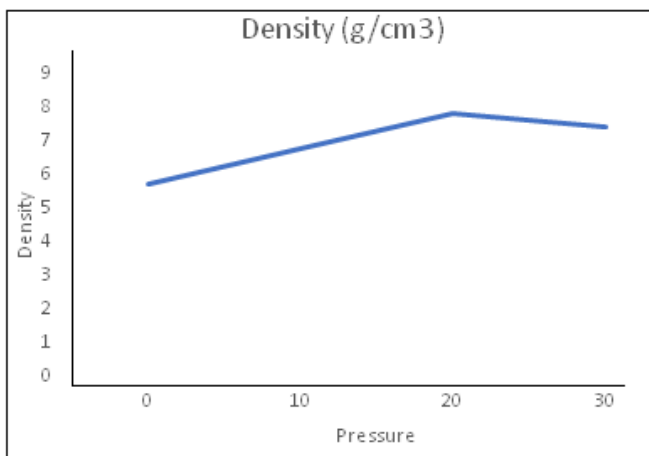**Fig 3.** Volume versus pressure for YBCO Superconductor

Fig 4. Density versus Pressure for YBCO Superconductor

is related with valence electron density (electron/unit volume). Higher the bulk modulus is result of concentration of electrons so it gives the high repulsive forces. At a fixed volume, Shear modulus measures the resistance to shape change. It is related to bond bending, and depends on the direction and plane of shear. The shear modulus and bulk modulus are related by Poisson's ratio (n), which is the ratio between the transverse strains and longitude strains. The Bulk Modulus (B), Young modulus (E), Shear modulus (G) and Poisson ratio (n) are calculated at different pressures for YBCO superconductor (Figures 5, 6, 7, 8 and 9) using Voigt Approximation, Reuss Approximation and Hill approximation.
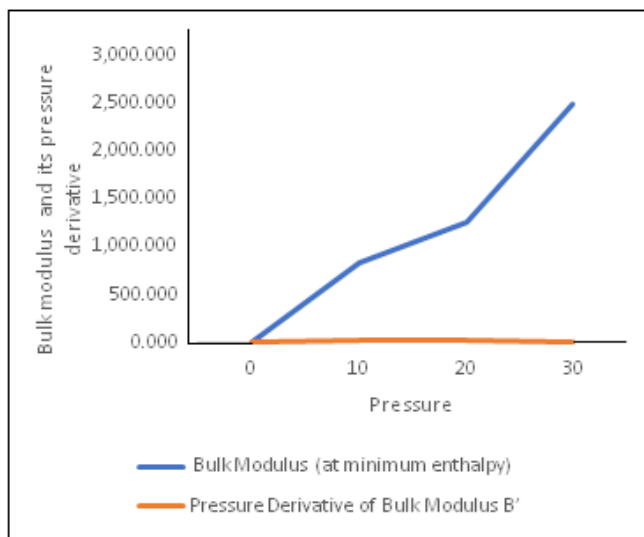

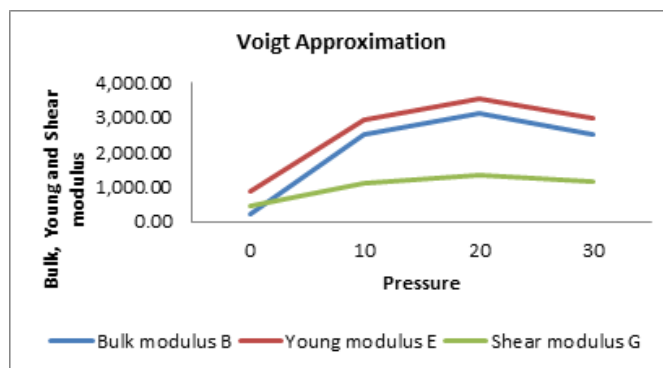**Fig 5.** Bulk modulus versus pressure for YBCO superconductor

Fig 6. Bulk, Young and Shear modulus versus pressure for YBCO superconductor

The corresponding calculated values of these parameters are given in Tables 2, 3 and 4. The bulk modulus and pressure derivative of bulk modulus have been increases with increasing the pressure for YBCO Superconductor.

The Bulk modulus(B),Young modulus(E),and Shear modulus(G) have been increases with increasing pressure by using voigt approximation, bulk modulus(B) decrease, young modulus(E) and shear modulus(G) have been increases with increasing pressure by using Reuss approximation and bulk modulus (B),young modulus(E) and shear modulus(G) have been increase with increasing the pressure by using Hill approximation. The Poisson's ratio decreases with increasing pressure by using voigt and Reuss approximation and increases with increasing pressure by using Hill approximation. The sound velocities have been calculated at different pressures and the sound velocities versus pressure graph is plotted for YBCO superconductor is represented in Figure 10.

Hill (13) (1952) shows, the Voigt- Reuss –hill average sound velocities are increases with pressure (14; 15) (Voigt, 1928;
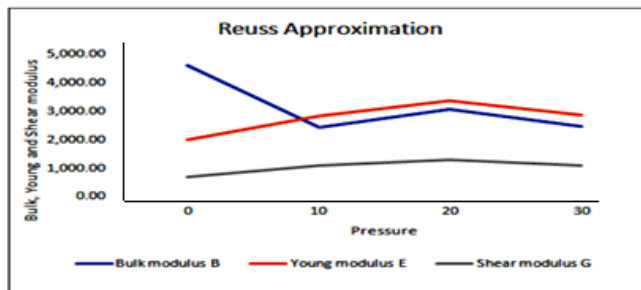
Fig 7. Bulk, Young, Shear modulus versus pressure for YBCO Superconductor
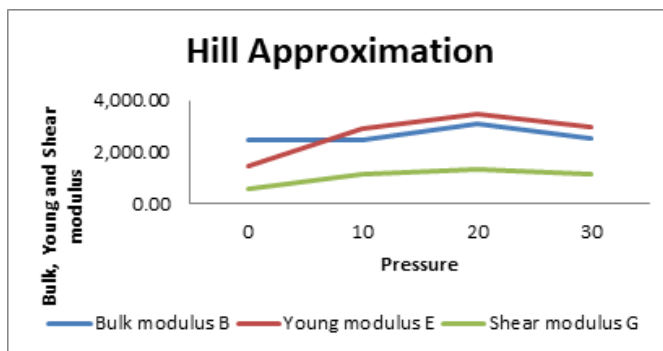
Fig 8. Bulk, Young, Shear modulus versus pressure for YBCO Superconductor
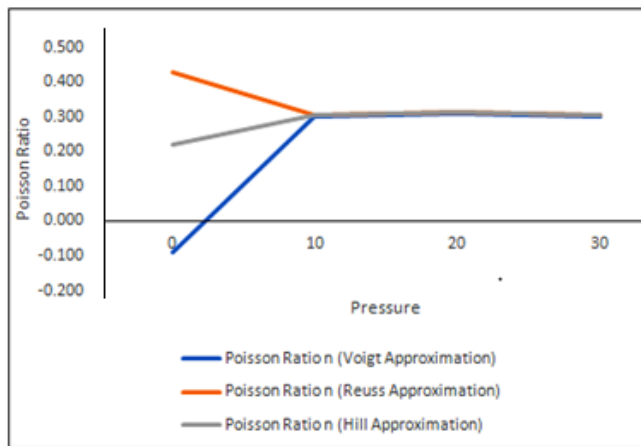

Fig 9. Poisson's ratios versus pressure for YBCO superconductor

Table 2. Calculated Values of Bulk modulus at minimum enthalpy and its pressure derivative

Pressure(GPa)	Bulk Modulus(B) (at minimum enthalpy)	Pressure derivative of Bulk Modulus (B)
0	0.000	1.113
10	830.94	15.000
20	1255.93	15
30	2,494.28	3.158

Table 3. Calculate Values of Bulk, Young and Shear modulii using different approximations for YBa$_2$Cu$_3$O$_7$

	Voigt approximation			Reuss approximation			Hill approximation		
Pressure (GPa)	Bulk modulus (B)	Young modulus (E)	Shear modulus (G)	Bulk modulus (B)	Young modulus (E)	Shear modulus (G)	Bulk modulus (B)	Young modulus (E)	Shear modulus (G)
0	241.97	857.69	471.65	4,639.15	2,014.01	705.36	2,440.56	1,435.85	588.51
10	2,497.47	2,947.88	1,130.95	2,456.56	2,837.14	1,084.94	2,477.01	2,892.51	1,107.94
20	3,112.85	3,541.10	1,351.15	3,072.39	3,398.95	1,291.77	3,092.62	3,470.02	1,321.46

Table 4. Calculate Values of Poisson Ratio using different approximations

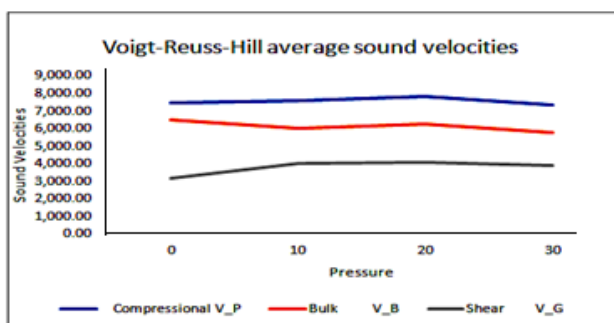| Pressure (GPa)	Poisson Ratio (n) (Voigt Approximation)	Poisson Ratio (n) (Reuss Approximation)	Poisson Ratio (n) (Hill Approximation)
0	-0.091	0.428	0.220
10	0.303	0.308	0.305
20	0.310	0.316	0.313
30	0.302	0.306	0.304

Fig 10. Sound velocities versus pressure for YBCO superconductor

Reuss, 1929) .The Approximate Debye temperature, Average Debye sound velocity, Debye temperature and Pugh's ratio(B/G) of YBa2Cu307 under pressure up to 30Gpa have been calculated and the results are summarized in table (5) and the corresponding values versus pressure for YBa2Cu3O7 plotted graphs are shown in Figure 11.

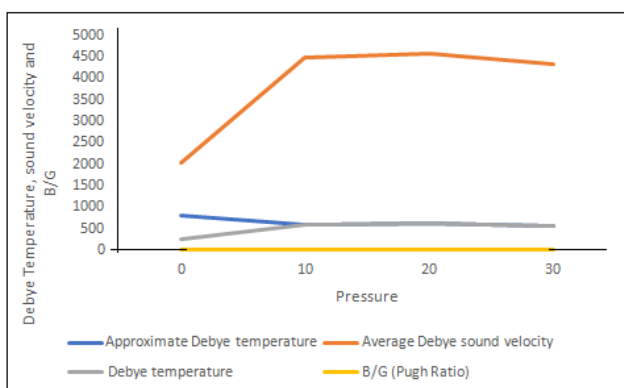**Fig 11.** Debye Temperature, Sound velocity and Pugh Ratio(B/G) versus Pressure for YBCO

Debye sound velocity(ϑ_D), Debye temperature(θ_D) increases with increasing pressure and Pugh's ratio(B/G) decreases with

increasing the pressure. The parameter B/G is known as the Pugh's ratio (B/G), which distinguishes between ductile and brittle response of YBCO Superconductor under applied stress. The Pugh's ratio (B/G) critical value is estimated to be 1.75 and larger value indicates ductile behavior. Another criterion often used to differentiate between ductile and brittle behavior is the Poisson's ratio (n). Poisson's ratio (n) greater than 0.26 implies the ductile behavior and we have obtained the Debye temperature. Both Pugh's ratio (B/G) and Poisson's ratio (n) predict moderately ductile response to stress for YBCO Superconductor.

4 Summary and Conclusion

In summary, High-pressure studies provide otherwise unattainable information about the phase diagrams, mechanical properties, and electronic structure which can predict directions for search of materials with desirable properties. Density Functional Theory (DFT) calculations using Quantum ESPRESSO under high pressure increasing systematically have been calculated and performed for YBCO up to 30Gpa. The lattice constants, Bulk modulus (B), Young modulus (E), Shear modulus (S) and Poisson ratio (n) versus pressure for YBCO Superconductor have been calculated in research this work. It has been shown that the Poisson's ratio decreases with increasing pressure by using voigt and Reuss approximation and increases with increasing pressure by using Hill approximation. The Sound velocities and Pugh's ratio (B/G) have been calculated for YBCO Superconductor. It was found that the Pugh's ratio (B/G), which distinguishes between ductile and brittle response of YBCO Superconductor under applied stress. The Pugh's ratio (B/G) critical value is estimated to be 1.75 and larger value indicates ductile behavior. Both Pugh's ratio (B/G) and Poisson's ratio (n) predict moderately ductile response to stress for YBCO Superconductor. The Pugh's ratio has been calculated at different pressures. Debye temperature increases with increasing pressure and Pugh's ratio (B/G) decreases with increasing the pressure.

Acknowledgements

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